



**AUSTRALIAN ATOMIC ENERGY COMMISSION
RESEARCH ESTABLISHMENT
LUCAS HEIGHTS**

**ANISOTROPIC COLLISION PROBABILITIES FOR
ONE DIMENSIONAL GEOMETRIES**

by

G. DOHERTY

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ABSTRACT

The equations for P_0 and P_1 collision probabilities in slab, spherical and cylindrical geometries are presented. A method of solution of the resulting multigroup neutron flux equation is discussed. The extension of S_n codes to incorporate anisotropic scattering is straightforward and the time penalty incurred in the calculation of the P_1 flux and source is small. The corresponding extension of the collision probability method is difficult and doubling the length of the flux vector increases the solution time dramatically. It is therefore concluded that the S_n method will be superior for most anisotropic calculations.

We regret that some of the pages in the microfiche copy of this report may not be up to the proper legibility standards, even though the best possible copy was used for preparing the master fiche.

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1. INTRODUCTION

The use of P_0 collision probabilities in cell calculations is widespread, even for systems where the method is competing directly with a one dimensional S_n alternative. The extension of the S_n approach to include P_1 scattering is relatively simple and involves a time penalty of something less than a factor of two. In this report we consider the extension of the collision probability method to include P_1 scattering for these one dimensional systems. It will be apparent that the collision probability calculation suffers badly by comparison, both in the additional complexity and in the time penalty incurred.

Slab geometry is discussed in Section 2. This geometry is unique in that the usual flat flux assumption, applied now to all the Legendre components of the flux, allows the computation of the P_n to P_n transfer matrix with the same ease as the P_0 to P_0 term. In fact since both involve the same exponentials in their evaluation, the additional transfer matrices are obtained for very little extra computational effort. In spherical geometry the curvature forces us to make a further approximation so that the P_n to P_n terms can be computed from the same exponentials as those required for the P_0 to P_0 terms. These results are presented in Section 3. Finally, for cylindrical geometry which is discussed in Section 4, we are forced to make a similar approximation to express our transfer matrices in a tractable form. Despite this approximation the computation of the higher components requires additional functions not needed in the evaluation of the P_0 terms and the time penalty is more severe.

In Section 5 we discuss a method of solution of the multigroup flux equations. This follows in essence the method used for the solution of the P_0 equations but because we are solving matrix equations of higher dimension there is again a substantial time penalty. The implication of these time penalties is that the collision probability calculations will be used mainly to obtain spectra suitable for group condensation. The formulae required in the group condensation procedure are presented in Section 6.

In Section 7 the results of different types of P_1 calculation are discussed. The general conclusions are that the P_0 approximation is adequate for cell calculations and that P_1 scattering should be included in criticality calculations of small water systems. The use of S_n codes is preferred to the collision probability alternative for this type of problem.

2. SLAB GEOMETRY

We begin with the multigroup form of the integral neutron transport equation

$$\phi_g(\underline{r}, \underline{\Omega}) = \int d\underline{y} \exp \left[- \int_0^y dt \Sigma_g(\underline{r} - \underline{\Omega} t) \right] \{ S_g(\underline{r} - \underline{\Omega} y, \underline{\Omega}) + \text{Sum}_{g'} \int d\underline{\Omega}' \Sigma_{g'g}(\underline{r} - \underline{\Omega} y, \underline{\Omega}' \rightarrow \underline{\Omega}) \phi_{g'}(\underline{r} - \underline{\Omega} y, \underline{\Omega}') \}, \quad (2.1)$$

where

- $\phi_g(\underline{r}, \underline{\Omega})$ is the group g angular flux at \underline{r} in direction $\underline{\Omega}$
- $\Sigma_g(\underline{r})$ is the group g total cross section of the material at \underline{r}
- $S_g(\underline{r}, \underline{\Omega})$ is the group g angular source at \underline{r} in direction $\underline{\Omega}$ (and may include a fission source which is flux dependent)
- $\Sigma_{g'g}(\underline{r}, \underline{\Omega}' \rightarrow \underline{\Omega})$ is the scattering cross section from group g' , direction $\underline{\Omega}'$, to group g , direction $\underline{\Omega}$ for the material at \underline{r}
- $\exp \left[- \int_0^y dt \Sigma_g(\underline{r} - \underline{\Omega} t) \right]$ is the transmission probability for a neutron born in group g at $\underline{r} - \underline{\Omega} y$ and travelling to \underline{r} .

Define θ to be the angle between $\underline{\Omega}$ and the normal to the slab interfaces and ψ to be the polar angle. The flux $\phi(\underline{\Omega})$ does not depend on ψ so we may consider

$$\phi_g(\underline{r}, \mu) = \int_0^{2\pi} d\psi \phi_g(\underline{r}, \underline{\Omega}) \quad (2.2)$$

with $\mu = \cos \theta$.

Thus Equation 2.1 can be rewritten

$$\begin{aligned} \phi_g(\underline{r}, \mu) = & \int dy \left[\exp - \int_0^y dt \Sigma_g(\underline{r} - \underline{\Omega}t) \right] \int_0^{2\pi} d\psi \{ S_g(\underline{r} - \underline{\Omega}y, \underline{\Omega}) + \\ & \text{Sum}_{g'} \int d\underline{\Omega}' \Sigma_{g'g}(\underline{r} - \underline{\Omega}y, \underline{\Omega}' - \underline{\Omega}) \phi_g(\underline{r} - \underline{\Omega}y, \underline{\Omega}') \} . \end{aligned} \quad (2.3)$$

The scattering cross section $\Sigma_{g'g}(\underline{r}, \underline{\Omega}' - \underline{\Omega})$ can be approximated by the Legendre polynomial expansion

$$\Sigma_{g'g}(\underline{r}, \underline{\Omega}' - \underline{\Omega}) = \text{Sum}_{\ell} \Sigma_{g'g\ell} \frac{2\ell+1}{4\pi} P_{\ell}(\underline{\Omega}' \cdot \underline{\Omega}) . \quad (2.4)$$

Now we make use of the addition theorem for Legendre polynomials

$$P_{\ell}(\underline{\Omega}' \cdot \underline{\Omega}) = P_{\ell}(\mu') P_{\ell}(\mu) + 2 \text{Sum}_{m=1}^{\ell} \frac{(\ell-m)!}{(\ell+m)!} P_{\ell}^m(\mu') P_{\ell}^m(\mu) \cos m(\psi' - \psi) \quad (2.5)$$

to obtain a considerable simplification of the scattering term in Equation 2.3. Thus

$$\int_0^{2\pi} d\psi \text{Sum}_{\ell} \frac{2\ell+1}{4\pi} P_{\ell}(\underline{\Omega}' \cdot \underline{\Omega}) = \text{Sum}_{\ell} \frac{2\ell+1}{2} P_{\ell}(\mu') P_{\ell}(\mu) . \quad (2.6)$$

Substituting into Equation 2.3 we obtain

$$\begin{aligned} \phi_g(\underline{r}, \mu) = & \int dy \exp \left[- \int_0^y dt \Sigma_g(\underline{r} - \underline{\Omega}t) \right] \{ S_g(\underline{r} - \underline{\Omega}y, \mu) \\ & + \text{Sum}_{g'} \text{Sum}_{\ell} \int d\mu' \Sigma_{g'g\ell} \frac{2\ell+1}{2} P_{\ell}(\mu') P_{\ell}(\mu) \phi_g(\underline{r} - \underline{\Omega}y, \mu') \} . \end{aligned} \quad (2.7)$$

The flux $\phi_g(\underline{r}, \mu)$ and the source $S_g(\underline{r}, \mu)$ can be expanded in a series of Legendre polynomials in μ .

$$\phi_g(\underline{r}, \mu) = \text{Sum}_{\ell} \frac{2\ell+1}{2} \phi_{g\ell}(\underline{r}) P_{\ell}(\mu) \quad (2.8)$$

$$S_g(\underline{r}, \mu) = \text{Sum}_{\ell} \frac{2\ell+1}{2} S_{g\ell}(\underline{r}) P_{\ell}(\mu) . \quad (2.9)$$

The coefficients of the expansions may be obtained from the orthogonality of the Legendre polynomials

$$\phi_{g\ell}(\underline{r}) = \int_{-1}^{+1} d\mu P_{\ell}(\mu) \phi_g(\underline{r}, \mu) \quad (2.10)$$

$$S_{g\ell} = \int_{-1}^{+1} d\mu P_{\ell}(\mu) S_g(\underline{r}, \mu) . \quad (2.11)$$

Inserting the expansions into Equation 2.7 and integrating yields the following result

$$\begin{aligned} \phi_{g\ell}(\underline{r}) = & \int_{-1}^{+1} d\mu P_{\ell}(\mu) \int dy \exp \left[- \int_0^y dt \Sigma_g(\underline{r} - \underline{\Omega}t) \right] \left\{ \text{Sum}_m \frac{2m+1}{2} S_{gm}(\underline{r} - \underline{\Omega}y) + \right. \\ & \left. \text{Sum}_{g'} \text{Sum}_{\ell'} \int_{-1}^{+1} d\mu' \Sigma_{g'g\ell'} \frac{2\ell'+1}{2} P_{\ell'}(\mu') P_{\ell'}(\mu) \text{Sum}_m \frac{2m+1}{2} \phi_{gm}(\underline{r} - \underline{\Omega}y) P_m(\mu') \right\} \\ = & \text{Sum}_m \frac{2m+1}{2} \int_{-1}^{+1} d\mu P_{\ell}(\mu) \int dy \exp \left[- \int_0^y dt \Sigma_g(\underline{r} - \underline{\Omega}t) \right] \left\{ S_{gm}(\underline{r} - \underline{\Omega}y) + \right. \\ & \left. \text{Sum}_{g'} \Sigma_{g'gm} \phi_{g'm}(\underline{r} - \underline{\Omega}y) \right\} P_m(\mu) . \end{aligned} \quad (2.12)$$

For slab geometry we replace the variables \underline{r} , y and $\underline{\Omega}$ by x , x' , μ .

Equation 2.12 becomes:

$$\begin{aligned} \phi_{g\ell}(x) = & \text{Sum}_m \frac{2m+1}{2} \int_{-1}^{+1} d\mu P_{\ell}(\mu) \int \frac{dx'}{\mu} \exp \left[- \frac{1}{|\mu|} \int_{x'}^x dt \Sigma_g(t) \right] \\ & \left\{ S_{gm}(x') + \text{Sum}_{g'} \Sigma_{g'gm} \phi_{g'm}(x') \right\} P_m(\mu) . \end{aligned} \quad (2.13)$$

In the spirit of the collision probability approach we assume $\phi_{g\ell}(x)$ is independent of x within regions R_i with volumes V_i and define, for these regions, the following quantities:

$$\phi_{ig\ell} = \int_{R_i} dx \phi_{g\ell}(x) / V_i \quad (2.14)$$

$$\Sigma_{ig} = \Sigma_g(x) \text{ for } x \text{ in } R_i \quad (2.15)$$

and
$$S_{igm} = S_{gm}(x) \text{ for } x \text{ in } R_i \quad (2.16)$$

Substituting into Equation 2.13 and integrating over R_i gives us

$$V_i \phi_{ig\ell} = \text{Sum}_j V_j \text{Sum}_m Q_{ijg\ell m} [S_{jgm} + \text{Sum}_{g'} \Sigma_{j'g'm} \phi_{j'g'm}] \quad (2.17)$$

with the transfer matrix Q defined by

$$Q_{ijg\ell m} = \frac{2m+1}{2V_j} \int_{-1}^{+1} P_{\ell}(\mu) P_m(\mu) \int_{R_j} \frac{dx'}{\mu} \int_{R_i} dx \exp \left[- \frac{1}{|\mu|} \int_{x'}^x \Sigma_g(t) dt \right] \quad (2.18)$$

The isotropic approximation commonly used in collision probability calculations simply truncates the summation over m in Equation 2.17 at the first term $m=0$. It is conventional when using this approximation to replace the total cross section appearing in Equation 2.18 by the transport cross section $\Sigma - \bar{\mu} \Sigma_s$. The correction has its origins in one group theory but is commonly applied to the multigroup situation where the justification for its use is purely empirical. In this report we will confine our attention to the P_1 approximation where the $m=0$ and $m=1$ terms are kept in the summation of Equation 2.17. It will be evident that the method can easily be extended to retain more terms in the sum, but in practice P_1 should be adequate for cell calculations. We postpone to Section 5 a discussion of the methods of solving Equation 2.17 and confine our attention at this stage to the calculations required in Equation 2.18.

The group index g is dropped on the understanding that the calculation will be repeated for each group.

$$Q_{ij\ell m} = \frac{2m+1}{2V_j} \int_{-1}^{+1} d\mu P_\ell(\mu) P_m(\mu) \int_{R_i} \frac{dx'}{\mu} \int_{R_i} dx \exp\left[-\frac{1}{|\mu|} \int_{x'}^x \Sigma(t) dt\right] \quad (2.19)$$

$$\text{Writing } T_i = \exp(-\Sigma_i x_i / \mu) \quad (2.20)$$

$$\text{and } u = \prod_{i=1}^k T_i \quad (2.21)$$

we obtain the following results.

Periodic Cell

For a k -slab periodic cell:

$$Q_{11\ell m} = \frac{2m+1}{2x_1} \int_0^1 d\mu [P_\ell(\mu) P_m(\mu) + P_\ell(-\mu) P_m(-\mu)] \left\{ \frac{x_1}{\Sigma_1} - \frac{\mu}{\Sigma_1^2} [1-T_1] \left[1 - \frac{(1-T_1)T_2 \dots T_k}{1-u} \right] \right\} \quad (2.22)$$

$$Q_{21\ell m} = \frac{2m+1}{2x_1} \int_0^1 d\mu P_\ell(\mu) P_m(\mu) \frac{\mu [1-T_1] [1-T_2]}{\Sigma_1 \Sigma_2 [1-u]} + \frac{2m+1}{2x_1} \int_0^1 d\mu P_\ell(-\mu) P_m(-\mu) \frac{\mu [1-T_1] T_3 \dots T_k [1-T_2]}{\Sigma_1 \Sigma_2 [1-u]} \quad (2.23)$$

$$Q_{j1\ell m} = \frac{2m+1}{2x_1} \int_0^1 d\mu P_\ell(\mu) P_m(\mu) \frac{\mu [1-T_1] T_2 \dots T_{j-1} [1-T_j]}{\Sigma_1 \Sigma_j [1-u]} + \frac{2m+1}{2x_1} \int_0^1 d\mu P_\ell(-\mu) P_m(-\mu) \frac{\mu [1-T_1] T_{j+1} \dots T_k [1-T_j]}{\Sigma_1 \Sigma_j [1-u]} \quad (2.24)$$

$$Q_{k1\ell m} = \frac{2m+1}{2x_1} \int_0^1 d\mu P_\ell(\mu) P_m(\mu) \frac{\mu [1-T_1] T_2 \dots T_{k-1} [1-T_k]}{\Sigma_1 \Sigma_k [1-u]} + \frac{2m+1}{2x_1} \int_0^1 d\mu P_\ell(-\mu) P_m(-\mu) \frac{\mu [1-T_1] [1-T_k]}{\Sigma_1 \Sigma_k [1-u]} \quad (2.25)$$

Equations for neutrons originating in slabs other than the first can be deduced by relabelling the slabs. To cut down the amount of calculation we can employ the following reciprocity relations:

$$(2\ell+1) Q_{ji\ell m} = (2m+1) Q_{jim\ell} \quad (2.26)$$

$$V_i Q_{ji\ell m} = (-1)^{\ell+m} V_j Q_{ij\ell m} \quad (2.27)$$

These equations may be established by writing down the explicit forms of the appropriate elements. Equation 2.27 with $\ell=m=0$ is the usual reciprocity relation found in isotropic collision probability theory.

Reflected Cell

For a k -slab cell reflected at left and right hand boundaries the explicit transfer elements are as follows:

$$Q_{11\ell m} = \frac{2m+1}{2x_1} \int_0^1 d\mu \left[P_\ell(\mu) P_m(\mu) \left\{ \frac{x_1}{\Sigma_1} - \frac{\mu [1-T_1]}{\Sigma_1^2} + \frac{\mu T_1 T_2^2 \dots T_k^2 [1-T_1]^2}{\Sigma_1^2 [1-u^2]} \right\} + P_\ell(-\mu) P_m(\mu) \frac{\mu T_2^2 \dots T_k^2 [1-T_1]^2}{\Sigma_1^2 [1-u^2]} + P_\ell(\mu) P_m(-\mu) \frac{\mu [1-T_1^2]}{\Sigma_1^2 [1-u^2]} + P_\ell(-\mu) P_m(-\mu) \left\{ \frac{x_1}{\Sigma_1} - \frac{\mu [1-T_1]}{\Sigma_1^2} + \frac{\mu T_1 T_2^2 \dots T_k^2 [1-T_1]^2}{\Sigma_1^2 [1-u^2]} \right\} \right] \quad (2.28)$$

$$Q_{21\ell m} = \frac{2m+1}{2x_1} \int_0^1 d\mu \left[P_\ell(\mu) P_m(\mu) \frac{\mu [1-T_1] [1-T_2]}{\Sigma_1 \Sigma_2 [1-u^2]} + P_\ell(-\mu) P_m(\mu) \frac{\mu [1-T_1] T_2 T_3^2 \dots T_k^2 [1-T_2]}{\Sigma_1 \Sigma_2 [1-u^2]} + P_\ell(\mu) P_m(-\mu) \frac{\mu [1-T_1] T_1 [1-T_2]}{\Sigma_1 \Sigma_2 [1-u^2]} + P_\ell(-\mu) P_m(-\mu) \frac{\mu [1-T_1] T_1 T_2 T_3^2 \dots T_k^2 [1-T_2]}{\Sigma_1 \Sigma_2 [1-u^2]} \right] \quad (2.29)$$

$$Q_{j1\ell m} = \frac{2m+1}{2x_1} \int_0^1 d\mu \left[P_\ell(\mu) P_m(\mu) \frac{\mu [1-T_1] T_2 \dots T_{j-1} [1-T_j]}{\Sigma_1 \Sigma_j [1-u^2]} + P_\ell(-\mu) P_m(\mu) \frac{\mu [1-T_1] T_2 \dots T_k T_k \dots T_{j+1} [1-T_j]}{\Sigma_1 \Sigma_j [1-u^2]} + P_\ell(\mu) P_m(-\mu) \frac{\mu [1-T_1] T_1 \dots T_{j-1} [1-T_j]}{\Sigma_1 \Sigma_j [1-u^2]} + P_\ell(-\mu) P_m(-\mu) \frac{\mu [1-T_1] T_1 \dots T_k T_k \dots T_{j+1} [1-T_j]}{\Sigma_1 \Sigma_j [1-u^2]} \right] \quad (2.30)$$

$$\begin{aligned}
Q_{k_1 l m} = & \frac{2m+1}{2x_i} \int_0^1 d\mu \left[P_\ell(\mu) P_m(\mu) \frac{\mu [1-T_1] T_2 \dots T_{k-1} [1-T_k]}{\Sigma_1 \Sigma_k [1-u^2]} \right. \\
& + P_\ell(-\mu) P_m(\mu) \frac{\mu [1-T_1] T_2 \dots T_k [1-T_k]}{\Sigma_1 \Sigma_k [1-u^2]} \\
& + P_\ell(\mu) P_m(-\mu) \frac{\mu [1-T_1] T_1 \dots T_{k-1} [1-T_k]}{\Sigma_1 \Sigma_k [1-u^2]} \\
& \left. + P_\ell(-\mu) P_m(-\mu) \frac{\mu [1-T_1] T_1 \dots T_k [1-T_k]}{\Sigma_1 \Sigma_k [1-u^2]} \right] \quad (2.31)
\end{aligned}$$

$$\begin{aligned}
Q_{i+1, i l m} = & \frac{2m+1}{2x_i} \int_0^1 d\mu \left[P_\ell(\mu) P_m(\mu) \frac{\mu [1-T_i] [1-T_{i+1}]}{\Sigma_i \Sigma_{i+1} [1-u^2]} \right. \\
& + P_\ell(-\mu) P_m(\mu) \frac{\mu [1-T_i] T_{i+1} \dots T_k T_{k+1} \dots T_{i+2} [1-T_{i+1}]}{\Sigma_i \Sigma_{i+1} [1-u^2]} \\
& + P_\ell(\mu) P_m(-\mu) \frac{\mu [1-T_i] T_{i-1} \dots T_1 T_1 \dots T_i [1-T_{i+1}]}{\Sigma_i \Sigma_{i+1} [1-u^2]} \\
& \left. + P_\ell(-\mu) P_m(-\mu) \frac{\mu [1-T_i] T_{i-1} \dots T_1 T_1 \dots T_k T_{k+1} \dots T_{i+2} [1-T_{i+1}]}{\Sigma_i \Sigma_{i+1} [1-u^2]} \right] \quad (2.32)
\end{aligned}$$

$$\begin{aligned}
Q_{j i l m} = & \frac{2m+1}{2x_i} \int_0^1 d\mu \left[P_\ell(\mu) P_m(\mu) \frac{\mu [1-T_i] T_{i+1} \dots T_{j-1} [1-T_j]}{\Sigma_i \Sigma_j [1-u^2]} \right. \\
& + P_\ell(-\mu) P_m(\mu) \frac{\mu [1-T_i] T_{i+1} \dots T_k T_{k+1} \dots T_{j+1} [1-T_j]}{\Sigma_i \Sigma_j [1-u^2]} \\
& + P_\ell(\mu) P_m(-\mu) \frac{\mu [1-T_i] T_{i-1} \dots T_1 T_1 \dots T_{j-1} [1-T_j]}{\Sigma_i \Sigma_j [1-u^2]} \\
& \left. + P_\ell(-\mu) P_m(-\mu) \frac{\mu [1-T_i] T_{i-1} \dots T_1 T_1 \dots T_k T_{k+1} \dots T_{j+1} [1-T_j]}{\Sigma_i \Sigma_j [1-u^2]} \right] \quad (2.33)
\end{aligned}$$

$$\begin{aligned}
Q_{k i l m} = & \frac{2m+1}{2x_i} \int_0^1 d\mu \left[P_\ell(\mu) P_m(\mu) \frac{\mu [1-T_i] T_{i+1} \dots T_{k-1} [1-T_k]}{\Sigma_i \Sigma_k [1-u^2]} \right. \\
& + P_\ell(-\mu) P_m(\mu) \frac{\mu [1-T_i] T_{i+1} \dots T_k [1-T_k]}{\Sigma_i \Sigma_k [1-u^2]} \\
& + P_\ell(\mu) P_m(-\mu) \frac{\mu [1-T_i] T_{i-1} \dots T_1 T_1 \dots T_{k-1} [1-T_k]}{\Sigma_i \Sigma_k [1-u^2]} \\
& \left. + P_\ell(-\mu) P_m(-\mu) \frac{\mu [1-T_i] T_{i-1} \dots T_1 T_1 \dots T_k [1-T_k]}{\Sigma_i \Sigma_k [1-u^2]} \right] \quad (2.34)
\end{aligned}$$

Unfortunately the reciprocity relation 2.26 no longer holds for the doubly reflected slab system. However Equation 2.27 remains valid except for the set $i = j, \ell \neq m$.

Free Slabs

The results for free slabs are somewhat simpler

$$Q_{ii l m} = \frac{2m+1}{2x_i} \int_0^1 d\mu [P_\ell(\mu) P_m(\mu) + P_\ell(-\mu) P_m(-\mu)] \left[\frac{x_i}{\Sigma_i} - \frac{\mu(1-T_i)}{\Sigma_i^2} \right] \quad (2.35)$$

$$Q_{j i l m} (j > i) = \frac{2m+1}{2x_i} \int_0^1 d\mu P_\ell(\mu) P_m(\mu) \frac{\mu [1-T_i] T_{i+1} \dots T_{j-1} [1-T_j]}{\Sigma_i \Sigma_j} \quad (2.36)$$

$$Q_{j i l m} (j < i) = \frac{2m+1}{2x_i} \int_0^1 d\mu P_\ell(-\mu) P_m(-\mu) \frac{\mu [1-T_i] T_{i-1} \dots T_{j+1} [1-T_j]}{\Sigma_i \Sigma_j} \quad (2.37)$$

Both the reciprocity relations 2.26 and 2.27 can be used for the free slab system.

The computation involved in handling the P_1 terms is small. The integrals over μ are performed in the isotropic problem by Gauss Legendre quadrature and most of the time is spent in the evaluation of the exponential terms T_i . The portion of the integrand involving the T_i is independent of the values of ℓ and m so that we obtain the additional elements of the transfer matrix for only a few extra additions and multiplications.

3. SPHERICAL GEOMETRY.

Again we begin with the multi-group form of the integral neutron transport equation.

$$\begin{aligned}
\phi_B(\underline{r}, \underline{\Omega}) = & \int dy \exp \left[- \int_0^y dt \Sigma_B(\underline{r} - \underline{\Omega} t) \right] \{ S_B(\underline{r} - \underline{\Omega} y, \underline{\Omega}) \\
& + \text{Sum}_{g'} \int d\Omega' \Sigma_{B'}(\underline{r} - \underline{\Omega} y, \Omega' \rightarrow \underline{\Omega}) \phi_{B'}(\underline{r} - \underline{\Omega} y, \Omega') \} \quad (3.1)
\end{aligned}$$

Let $\hat{\underline{r}}$ be the unit radial vector through the point \underline{r} and

$$\mu = \hat{\underline{r}} \cdot \underline{\Omega} \quad (3.2)$$

Then if ψ is an angle in the plane normal to \hat{r} the symmetry of spherical geometry allows us to assert that the angular flux $\phi_s(\underline{r}, \underline{\Omega})$ is independent of ψ . Thus we may write, as in the slab situation

$$\phi_s(\underline{r}, \mu) = \int_0^{2\pi} d\psi \phi_s(\underline{r}, \underline{\Omega}) \quad (3.3)$$

The difference from the slab geometry is that μ in slab geometry is the cosine of the angle between $\underline{\Omega}$ and the normal to the slab interfaces and is independent of \underline{r} . In spherical geometry the track with direction $\underline{\Omega}$ passes through \underline{r} and $\underline{r} - \underline{\Omega}y$, and the μ for each point is different. We denote the value of μ at $\underline{r} - \underline{\Omega}y$ by μ' to distinguish it from the value at \underline{r} .

Again we expand the flux in Legendre polynomials in μ and repeat the steps for slab geometry. The space average flux is differently defined in spherical geometry

$$\phi_{ig\ell} = \int_{r_{i-1}}^{r_i} 4\pi r^2 \phi_{s\ell}(r) dr / V_i \quad (3.4)$$

and we use the relation

$$\phi_{s\ell}(r) = \phi_{ig\ell} \quad , \quad r_{i-1} < r < r_i \quad (3.5)$$

in the evaluation of integrals.

Thus after some manipulation, Equation 3.1 can be rewritten

$$V_i \phi_{ig\ell} = \int_{r_{i-1}}^{r_i} 4\pi r^2 dr \int_{-1}^{+1} d\mu P_\ell(\mu) \int dy \exp \left[- \int_0^y dt \Sigma_g(\underline{r} - \underline{\Omega}t) \right] \\ \text{Sum}_m \frac{2m+1}{2} P_m(\mu') \{ S_{gm}(\underline{r} - \underline{\Omega}y) + \text{Sum}_g \Sigma_{g'm} \phi_{g'm}(\underline{r} - \underline{\Omega}y) \} \quad (3.6)$$

We are trying to evaluate the transfer matrix $Q_{ijg\ell m}$ which satisfies the relation

$$V_i \phi_{ig\ell} = \text{Sum}_j V_j \text{Sum}_m Q_{ijg\ell m} [S_{jgm} + \text{Sum}_g \Sigma_{jg'm} \phi_{jg'm}] \quad (3.7)$$

Using Equation 3.6 we shall first examine $Q_{i1g\ell m}$ which is the transfer term for neutrons born in the central region ($r < r_1$) and colliding in region i ($r_{i-1} < r < r_i$). The index g is dropped on the understanding that the calculation is repeated for all groups. From geometric considerations it is obvious that the contribution to the integral over μ in Equation 3.6 is limited to the range $0 < \mu < \sqrt{1 - r_1^2/r^2}$. Thus

$$Q_{i1\ell m} = \frac{2m+1}{2V_1} \int_{r_{i-1}}^{r_i} 4\pi r^2 dr \int_{\sqrt{1-r_1^2/r^2}}^1 d\mu P_\ell(\mu) \int_{-\sqrt{r_1^2-r^2(1-\mu^2)}}^{+\sqrt{r_1^2-r^2(1-\mu^2)}} dy \\ \exp \{ - \Sigma_i [r\mu - \sqrt{r_{i-1}^2 - r^2(1-\mu^2)}] \} \\ \exp \{ - \Sigma_{i-1} [\sqrt{r_{i-1}^2 - r^2(1-\mu^2)} - \sqrt{r_{i-2}^2 - r^2(1-\mu^2)}] \} \\ \dots \exp \{ - \Sigma_1 [\sqrt{r_1^2 - r^2(1-\mu^2)} - y] \} P_m \left(\frac{y}{\sqrt{r^2(1-\mu^2) + y^2}} \right) \quad (3.8)$$

Changing variables to

$$x = r \sqrt{1-\mu^2} \quad (3.9)$$

$$z = r\mu \quad (3.10)$$

and defining

$$z_i = \sqrt{r_i^2 - x^2} \quad (3.11)$$

$$d_i = z_i - z_{i-1} \quad (3.12)$$

we can transform 3.8 to the simpler form

$$Q_{i1\ell m} = \frac{2m+1}{V_1} \int_0^{r_1} 2\pi x dx \exp \{ - [\Sigma_{i-1} d_{i-1} + \dots + \Sigma_2 d_2] \} \\ \int_{z_{i-1}}^{z_i} dz P_\ell \left(\frac{z}{\sqrt{z^2 + x^2}} \right) \exp [- \Sigma_i (z - z_{i-1})] \\ \int_{-z_1}^{z_1} dy P_m \left(\frac{y}{\sqrt{y^2 + x^2}} \right) \exp [- \Sigma_1 (z_1 - y)] \quad (3.13)$$

The integrals over z and y cannot be performed analytically except for the trivial case $\ell=m=0$. For the z integral we make the approximation

$$\int_{z_{i-1}}^{z_i} dz P_1 \left(\frac{z}{\sqrt{z^2 + x^2}} \right) \exp [- \Sigma_i (z - z_{i-1})] \\ = \frac{\sqrt{z_i^2 + x^2} - \sqrt{z_{i-1}^2 + x^2}}{z_i - z_{i-1}} \int_{z_{i-1}}^{z_i} dz \exp [- \Sigma_i (z - z_{i-1})] \\ = \frac{r_i - r_{i-1}}{z_i - z_{i-1}} [1 - \exp (- \Sigma_i d_i)] / \Sigma_i \\ = \mu_i [1 - \exp (- \Sigma_i d_i)] / \Sigma_i \quad (3.14)$$

The use of the same approximation for the y integral would give zero whatever the value of Σ_1 and we have therefore constructed a slightly more elaborate approximation for the central region

$$\int_{-z_1}^{z_1} dy P_1 \left(\frac{y}{\sqrt{y^2 + x^2}} \right) \exp [- \Sigma_1 (z_1 - y)] \\ = \frac{z_1}{\sqrt{z_1^2 + 4x^2}} \frac{1 - \exp (- \Sigma_1 z_1)}{1 + \exp (- \Sigma_1 z_1)} \frac{[1 - \exp (- 2 \Sigma_1 z_1)]}{\Sigma_1} \\ = \mu_1^* [1 - \exp (- 2 \Sigma_1 z_1)] / \Sigma_1 \quad (3.15)$$

The approximations 3.14 and 3.15 do introduce an error into the calculation of the collision probabilities which is small provided that the mesh intervals remain reasonably small. In fact the error introduced here is of the same order as that implicit in the flat flux assumption for if we were to assume a radial dependence of a + b $\sqrt{y^2 + x^2}$ for the flux components in each mesh interval we would have a term a + b $\sqrt{y^2 + x^2}$ appearing in the y integration. The distinction between slabs and spheres is most apparent at this point. In the slab problem the flat flux assumption is the only approximation in the evaluation of the anisotropic transfer matrix.

Returning to the calculation of more general elements in the transfer matrix we notice that contributions $Q_{i_2 l_m}$ consist of a term $Q_{i_2 l_m}^1$ arising from neutron tracks which cross region 1, and a term $Q_{i_2 l_m}^2$ from tracks which cross region 2 but pass outside region 1. For the term $Q_{i k l_m}$ there will be k such terms $Q_{i k l_m}^j$ with

$$Q_{i k l_m} = \sum_{j=1}^k Q_{i k l_m}^j \quad (3.16)$$

$$\text{Defining } T_j = \exp(-\sum_j d_j) \quad (3.17)$$

we may write down some of the elements of Q as follows:

$$Q_{i_1 l_m} = \frac{2m+1}{V_1} \int_0^{r_1} 2\pi x dx T_2 \dots T_{i-1} \int_{z_{i-1}}^{z_i} dz P_\ell(z/\sqrt{z^2+x^2}) \exp[-\sum_i(z-z_{i-1})] \int_{-z_1}^{z_1} dy P_m(y/\sqrt{y^2+x^2}) \exp[-\sum_1(z_1-y)] \quad (3.18)$$

$$Q_{i_2 l_m}^1 (i > 2) = \frac{2m+1}{V_2} \int_0^{r_1} 2\pi x dx T_3 \dots T_{i-1} \int_{z_{i-1}}^{z_i} dz P_\ell(z/\sqrt{z^2+x^2}) \exp[-\sum_i(z-z_{i-1})] \int_{z_1}^{z_2} dy \{ P_m(y/\sqrt{y^2+x^2}) \exp[-\sum_2(z_2-y)] + P_m(-y/\sqrt{y^2+x^2}) T_2 T_1^2 \exp[-\sum_2(y-z_1)] \} \quad (3.19)$$

$$Q_{i k l_m}^1 (i > k) = \frac{2m+1}{V_k} \int_0^{r_1} 2\pi x dx T_{k+1} \dots T_{i-1} \int_{z_{i-1}}^{z_i} dz P_\ell(z/\sqrt{z^2+x^2}) \exp[-\sum_i(z-z_{i-1})] \int_{z_{k-1}}^{z_k} dy \{ P_m(y/\sqrt{y^2+x^2}) \exp[-\sum_k(z_k-y)] + P_m(-y/\sqrt{y^2+x^2}) T_{k-1} \dots T_1 T_1 \dots T_k \exp[-\sum_k(y-z_{k-1})] \} \quad (3.20)$$

$$Q_{i k l_m}^j = \frac{2m+1}{V_k} \int_{r_{j-1}}^{r_j} 2\pi x dx T_{k+1} \dots T_{i-1} \int_{z_{i-1}}^{z_i} dz P_\ell(z/\sqrt{z^2+x^2}) \exp[-\sum_i(z-z_{i-1})] \int_{z_{k-1}}^{z_k} dy \{ P_m(y/\sqrt{y^2+x^2}) \exp[-\sum_k(z_k-y)] + P_m(-y/\sqrt{y^2+x^2}) T_{k-1} \dots T_j T_j \dots T_k \exp[-\sum_k(y-z_{k-1})] \} \quad (3.21)$$

$$Q_{i_1 l_m} = \frac{2m+1}{V_1} \int_0^{r_1} 2\pi x dx \int_{-z_1}^{z_1} dz P_\ell(z/\sqrt{z^2+x^2}) \int_{-z_1}^z dy P_m(y/\sqrt{y^2+x^2}) \exp[-\sum_1(z-y)] \quad (3.22)$$

$$Q_{k k l_m}^1 (i < k) = \frac{2m+1}{V_k} \int_{r_{j-1}}^{r_j} 2\pi x dx \left\{ \int_{z_{k-1}}^{z_k} dz P_\ell(-z/\sqrt{z^2+x^2}) \int_z^{z_k} dy P_m(-y/\sqrt{y^2+x^2}) \exp[-\sum_k(y-z)] + T_j^2 \dots T_{k-1}^2 \int_{z_{k-1}}^{z_k} dz P_\ell(z/\sqrt{z^2+x^2}) \exp[-\sum_k(z-z_{k-1})] \cdot \int_{z_{k-1}}^{z_k} dy P_m(-y/\sqrt{y^2+x^2}) \exp[-\sum_k(y-z_{k-1})] + \int_{z_{k-1}}^{z_k} dz P_\ell(z/\sqrt{z^2+x^2}) \int_{z_{k-1}}^z dy P_m(y/\sqrt{y^2+x^2}) \exp[-\sum_k(z-y)] \right\} \quad (3.23)$$

We have a reciprocity relation which restricts the explicit probability calculation to elements $Q_{ij l_m}$ with $i \geq j$. This relation remains true whether the approximations 3.14 and 3.15 or the exact expressions for the P_1 integrals are employed. The relation is

$$(2\ell+1) V_i Q_{j i l_m} = (-1)^{\ell+m} (2m+1) V_j Q_{i j l_m} \quad (j \neq i) \quad (3.24)$$

4. CYLINDRICAL GEOMETRY

In cylindrical geometry we perform a spherical harmonics expansion of the flux ϕ . Let θ be the angle between the direction of travel Ω and the z axis and let ψ be the angle between the radius \tilde{r} and the projection of Ω on the $z=0$ plane. If we confine our attention to systems with a cylindrical outer boundary then the flux $\phi_g(\tilde{r}, \Omega)$ is an even function of ψ and the expansion is limited to the even spherical harmonics.

$$Y_{\ell m}(\theta, \psi) = P_\ell^m(\cos \theta) \cos m\psi \quad (4.1)$$

These functions satisfy the orthogonality relation

$$\int_0^{2\pi} d\psi \int_0^\pi \sin \theta d\theta Y_{\ell m}(\theta, \psi) Y_{\ell' m'}(\theta, \psi) = \frac{4\pi}{(2-\delta_{\ell 0})(2\ell+1)} \left[\frac{(\ell-m)!}{(\ell+m)!} \right] \delta_{\ell\ell'} \delta_{mm'} \quad (4.2)$$

$$= \delta_{\ell\ell'} \delta_{mm'} / A_{\ell m}$$

which defines the normalisation factors $A_{\ell m}$.

The expansion of the flux then becomes

$$\phi_g(\underline{r}, \underline{\Omega}) = \sum_{\ell} \sum_{m=0}^{\ell} A_{\ell m} \phi_{g\ell m}(\underline{r}) Y_{\ell m}(\theta, \psi) \quad (4.3)$$

with

$$\phi_{g\ell m}(\underline{r}) = \int_0^{2\pi} d\psi \int_0^\pi \sin \theta d\theta Y_{\ell m}(\theta, \psi) \phi_g(\underline{r}, \underline{\Omega}) \quad (4.4)$$

The integral multigroup equation is (again)

$$\phi_g(\underline{r}, \underline{\Omega}) = \int dy \exp \left[-\int_0^y dt \Sigma_g(\underline{r}-\underline{\Omega}t) \right] \left\{ S_g(\underline{r}-\underline{\Omega}y, \underline{\Omega}) + \sum_{g'} \int d\Omega' \Sigma_{g'g}(\underline{r}-\underline{\Omega}y, \underline{\Omega}' \rightarrow \underline{\Omega}) \phi_{g'}(\underline{r}-\underline{\Omega}y, \underline{\Omega}') \right\} \quad (4.5)$$

Applying Equations 2.4 and 2.5 to the scattering term of Equation 4.5 we arrive at the result

$$\int d\Omega' \Sigma_{g'g}(\underline{r}-\underline{\Omega}y, \underline{\Omega}' \rightarrow \underline{\Omega}) \phi_{g'}(\underline{r}-\underline{\Omega}y, \underline{\Omega}') = \sum_{\ell} \sum_{g' \ell} \sum_{m=0}^{\ell} A_{\ell m} \phi_{g' \ell m} Y_{\ell m}(\theta, \psi') \quad (4.6)$$

where ψ' is the value of ψ at $\underline{r}-\underline{\Omega}y$. Because ψ is measured relative to the radius, its value is different at each point on the neutron track.

The source and scattering terms of Equation 4.5 can now be combined to obtain the form

$$\phi_g(\underline{r}, \underline{\Omega}) = \int dy \exp \left[-\int_0^y dt \Sigma_g(\underline{r}-\underline{\Omega}t) \right] \sum_{\ell} \sum_{m=0}^{\ell} A_{\ell m} Y_{\ell m}(\theta, \psi') \left[S_{g\ell m}(\underline{r}-\underline{\Omega}y) + \sum_{g'} \Sigma_{g'g\ell} \phi_{g' \ell m}(\underline{r}-\underline{\Omega}y) \right] \quad (4.7)$$

Substituting Equation 4.7 into Equation 4.4 gives us

$$\phi_{g\ell m}(\underline{r}) = \int_0^{2\pi} d\psi \int_0^\pi \sin \theta d\theta Y_{\ell m}(\theta, \psi) \int dy \exp \left[-\int_0^y dt \Sigma_g(\underline{r}-\underline{\Omega}t) \right] \sum_p \sum_{q=0}^p A_{pq} Y_{pq}(\theta, \psi') \left[S_{gpq}(\underline{r}-\underline{\Omega}y) + \sum_{g'} \Sigma_{g'gp} \phi_{g' pq}(\underline{r}-\underline{\Omega}y) \right] \quad (4.8)$$

Before proceeding further we shall restrict ourselves to the P_1 approximation so that the sum over p in Equation 4.8 is truncated at $p=1$. From Equation 4.1 we have

$$Y_{00}(\theta, \psi) = 1 \quad (4.9)$$

$$Y_{10}(\theta, \psi) = \cos \theta \quad (4.10)$$

$$Y_{11}(\theta, \psi) = \sin \theta \cos \psi \quad (4.11)$$

Now we note that Y_{10} is an odd function over the range $(0, \pi)$ of the θ integration of Equation 4.8 while both Y_{00} and Y_{11} are even functions. This implies that the only non-zero integrals involving Y_{10} will be those where $\ell=p=1$ and $m=q=0$. Since the values of ϕ_{g00} are completely independent of the ϕ_{g10} components it will be unnecessary to carry the latter through the rest of our analysis. Thus we may shorten our suffix notation and consider

$$Y_0 = Y_{00}, \quad Y_1 = Y_{11} \quad (4.12)$$

$$\phi_{g0} = \phi_{g00}, \quad \phi_{g1} = \phi_{g11}, \quad \text{etc.}$$

Thus Equation 4.8 can be rewritten

$$\phi_{g\ell}(\underline{r}) = \int_0^{2\pi} d\psi \int_0^\pi \sin \theta d\theta Y_{\ell}(\theta, \psi) \int dy \exp \left[-\int_0^y dt \Sigma_g(\underline{r}-\underline{\Omega}t) \right] \left[\sum_p A_p Y_p [S_{gp}(\underline{r}-\underline{\Omega}y) + \sum_{g'} \Sigma_{g'gp} \phi_{g'p}(\underline{r}-\underline{\Omega}y)] \right] \quad (4.13)$$

We define the usual average value

$$\phi_{ig\ell} = \int_{r_{i-1}}^{r_i} 2\pi r dr \phi_{g\ell}(\underline{r}) / V_i \quad (4.14)$$

and employ the flat flux assumption

$$\phi_{g\ell}(\underline{r}) = \phi_{ig\ell} \quad \text{for} \quad r_{i-1} < r < r_i \quad (4.15)$$

Substituting into Equation 4.13 and integrating over r gives

$$\phi_{ig\ell} = \int_{r_{i-1}}^{r_i} 2\pi r dr \int_0^{2\pi} d\psi \int_0^\pi \sin \theta d\theta Y_{\ell}(\theta, \psi) \int dy \exp \left[-\int_0^y dt \Sigma_g(\underline{r}-\underline{\Omega}t) \right] \left[\sum_p A_p Y_p(\theta, \psi') [S_{gp}(\underline{r}-\underline{\Omega}y) + \sum_{g'} \Sigma_{g'gp} \phi_{g'p}(\underline{r}-\underline{\Omega}y)] \right] \quad (4.16)$$

Thus again we are looking for the elements $Q_{ijg\ell m}$ which allow us to rewrite Equation 4.16 in the matrix form

$$\phi_{ig\ell} = \sum_j V_j \sum_m Q_{ijg\ell m} [S_{jgm} + \sum_{g'} \Sigma_{g'gm} \phi_{jg'm}] \quad (4.17)$$

We begin by examining Q_{i11m} which is the transfer term for neutrons born in the central region $r < r_1$ and arriving in region i where $r_{i-1} < r < r_i$. From geometric considerations it is obvious that the integration over ψ in Equation 4.16 is restricted to the range $-\pi_1/r < \sin \psi < \pi_1/r$.

Thus

$$\begin{aligned}
Q_{i1l_m} = & \frac{A_m}{V_1} \int_{r_{i-1}}^{r_i} 2\pi r dr \int_{-\sin^{-1}(r_1/r)}^{\sin^{-1}(r_1/r)} d\psi \int_0^\pi \sin\theta d\theta Y_l(\theta, \psi) \int_{-\sqrt{r_1^2 - r^2 \sin^2 \psi}}^{\sqrt{r_1^2 - r^2 \sin^2 \psi}} dy / \sin\theta \\
& \exp \{ -\Sigma_i [r \cos \psi - \sqrt{r_{i-1}^2 - r^2 \sin^2 \psi}] / \sin\theta \} \\
& \cdot \exp \{ -\Sigma_{i-1} [\sqrt{r_{i-1}^2 - r^2 \sin^2 \psi} - \sqrt{r_{i-2}^2 - r^2 \sin^2 \psi}] / \sin\theta \} \\
& \dots \exp \{ -\Sigma_1 [\sqrt{r_1^2 - r^2 \sin^2 \psi} - y] / \sin\theta \} Y_m(\theta, \tan^{-1}(r \sin \psi / y)) . \quad (4.18)
\end{aligned}$$

Changing variables to $x = r \sin \psi$, $z = \sqrt{r^2 - x^2}$ and defining

$$z_i = \sqrt{r_i^2 - x^2} \quad \text{and} \quad d_i = z_i - z_{i-1}$$

leads to a simpler form of Equation 4.18.

$$\begin{aligned}
Q_{i1l_m} = & \frac{2 A_m}{V_1} \int_{r_0}^{r_1} 2\pi x dx \int_0^\pi d\theta \exp \{ -[\Sigma_{i-1} d_{i-1} + \dots + \Sigma_2 d_2] / \sin\theta \} \\
& \int_{z_{i-1}}^{z_i} dz Y_l(\theta, \cos^{-1}(z / \sqrt{z^2 + x^2})) \exp \{ -\Sigma_i (z - z_{i-1}) / \sin\theta \} \\
& \int_{-z_1}^{z_1} dy Y_m(\theta, \cos^{-1}(y / \sqrt{y^2 + x^2})) \exp \{ -\Sigma_i (z_1 - y) / \sin\theta \} . \quad (4.19)
\end{aligned}$$

From the similarity between Equation 4.19 and Equation 3.13 the general terms for the other elements of Q in cylindrical geometry can easily be deduced, and we shall not bother to reproduce them here. Again we are forced to approximate the integrals over z and y for l or $m = 1$.

The approximations for the z integrals are:

$$\begin{aligned}
& \int_{z_{i-1}}^{z_i} dz Y_1(\theta, \cos^{-1}(z / \sqrt{z^2 + x^2})) \exp \{ -\Sigma_i (z - z_{i-1}) / \sin\theta \} \\
& \approx \frac{\sqrt{z_i^2 + x^2} - \sqrt{z_{i-1}^2 + x^2}}{z_i - z_{i-1}} \sin\theta \int_{z_{i-1}}^{z_i} dz \exp \{ -\Sigma_i (z - z_{i-1}) / \sin\theta \} \\
& = \frac{r_i - r_{i-1}}{z_i - z_{i-1}} \sin^2 \theta \{ 1 - \exp \{ -\Sigma_i (z_i - z_{i-1}) / \sin\theta \} \} \\
& = \mu_i \sin^2 \theta \{ 1 - \exp \{ -\Sigma_i (z_i - z_{i-1}) / \sin\theta \} \} \quad (4.20)
\end{aligned}$$

$$\begin{aligned}
& \int_{-z_1}^{z_1} dy Y_1(\theta, \cos^{-1}(y / \sqrt{y^2 + x^2})) \exp \{ -\Sigma_i (z_1 - y) / \sin\theta \} \\
& = \frac{z_1}{\sqrt{z_1^2 + 4x^2}} \frac{1 - \exp(-2\Sigma z_1)}{1 + \exp(-2\Sigma z_1)} \sin\theta \int_{-z_1}^{z_1} dz \exp \{ -\Sigma_i (z_1 - y) / \sin\theta \} \\
& = \mu_1^* \sin^2 \theta \{ 1 - \exp \{ -2\Sigma_1 d_1 / \sin\theta \} \} . \quad (4.21)
\end{aligned}$$

Takahashi (1966) has used a similar approximation in his code, FIRST II, though the z dependence of his average $\cos \psi$ is not explicitly stated. The approximation is evidently worse in cylindrical geometry than in spherical geometry because of the appearance of the $\sin \theta$ term in the exponential. However if we wish to obtain a form involving the Bickley functions

$$K_{in}(x) = \int_0^{\pi/2} \sin^2 \theta e^{-x/\sin\theta} d\theta , \quad (4.22)$$

we are forced into an approximation of this type.

From Equation 4.2 we see that $A_0 = 1/4\pi$ and $A_1 = 3/4\pi$.

Defining T_i by

$$T_i = \exp \{ -\Sigma_i (z_i - z_{i-1}) / \sin\theta \} , \quad (4.23)$$

we may write the various elements of Q_{i1l_m} as follows:

$$Q_{i100} = \frac{2}{V_1 \Sigma_1 \Sigma_i} \int_0^{r_1} dx \int_0^{\pi/2} \sin^2 \theta d\theta [1 - T_1^2] T_2 \dots T_{i-1} [1 - T_i] \quad (4.24)$$

$$Q_{i110} = \frac{2}{V_1 \Sigma_1 \Sigma_i} \int_0^{r_1} dx \mu_i \int_0^{\pi/2} \sin^3 \theta d\theta [1 - T_1^2] T_2 \dots T_{i-1} [1 - T_i] \quad (4.25)$$

$$Q_{i101} = \frac{6}{V_1 \Sigma_1 \Sigma_i} \int_0^{r_1} dx \mu_1^* \int_0^{\pi/2} \sin^3 \theta [1 - T_1^2] T_2 \dots T_{i-1} [1 - T_i] \quad (4.26)$$

$$Q_{i111} = \frac{6}{V_1 \Sigma_1 \Sigma_i} \int_0^{r_1} dx \mu_i \mu_1^* \int_0^{\pi/2} \sin^4 \theta [1 - T_1^2] T_2 \dots T_{i-1} [1 - T_i] . \quad (4.27)$$

It is obvious that these elements can be written in terms of the Bickley functions. Q_{i110} involves K_{i3} , both Q_{i101} and Q_{i110} involve K_{i4} , and Q_{i111} involves K_{i5} . The arguments in each case are the same. This means that the evaluation of the P_1 collision probability matrices requires about three times the computation time of that used in the usual isotropic calculation. Clearly the S_n method which involves very little extra computation to include P_1 scattering will be markedly superior in cylindrical geometry.

Again in cylindrical geometry the following reciprocity relation is valid

$$(2\ell+1) V_i Q_{ji\ell m} = (-1)^{\ell+m} (2m+1) V_j Q_{ijm\ell} \quad j \neq i . \quad (4.28)$$

Our discussion of the cylindrical system with a free outer boundary is now complete. The boundaries more commonly encountered in practical situations are either square or hexagonal and reflecting, both of which are replaced by a cylindrical one enclosing the same volume. From isotropic calculations we know that mirror reflection at the cylindrical boundary is a poor approximation and since the effect is geometric we may expect that the same condition in the P_1 calculation will be equally poor.

The alternative assumption which gives reasonable results in isotropic calculations is that the returning neutrons satisfy a $\sin \theta \cos \psi$ distribution. This implies that there is no correlation between the neutron directions before and after reflection at the boundary. At first glance such an approximation appears quite unsuitable for a P_1 calculation where we have endeavoured to follow the neutron direction carefully. However it has the virtue that it enables us to calculate the contribution of the reflected neutrons without difficulty and in any case cannot be a more drastic assumption than replacing the polygonal boundary by a cylindrical one.

Let $Q_{Bi\ell}$ be the transfer element for neutrons born with angular distribution ℓ in region i and reaching the boundary B without collision. Thus for the central region these elements are

$$Q_{B10} = \frac{2}{V_1 \Sigma_1} \int_0^{r_1} dx \int_0^{\pi/2} \sin^2 \theta [1 - T_1^2] T_2 \dots T_N \quad (4.29)$$

$$Q_{B11} = \frac{6}{V_1 \Sigma_1} \quad (4.30)$$

Let Q_{jBm} be the transfer element for neutrons born with distribution $\sin \theta \cos \psi$ on the boundary B and contributing to the flux component m in region j . Typical elements, again for the central region, are:

$$Q_{1B0} = (4/\pi r_N \Sigma_1) \int_0^{r_1} dx \int_0^{\pi/2} \sin^2 \theta [1 - T_1^2] T_2 \dots T_N \quad (4.31)$$

$$Q_{1B1} = (-4/\pi r_N \Sigma_1) \int_0^{r_1} dx \mu_1^* \int_0^{\pi/2} \sin^3 \theta [1 - T_1^2] T_2 \dots T_N \quad (4.32)$$

From these typical equations we deduce the general reciprocity relation

$$Q_{iB\ell} = \frac{(-1)^\ell 2 V_i}{(2\ell + 1) \pi r_N} Q_{Bi\ell} \quad (4.33)$$

We also require the quantity Q_{BB} which is the transfer element for neutrons born on the boundary B with distribution $\sin \theta \cos \psi$ and arriving uncollided again at the boundary B .

$$Q_{BB} = 1 - \sum_j \sum_i Q_{jBo} \quad (4.34)$$

The general transfer element $Q_{ij\ell m}$ for the reflected system is related to the free boundary term $Q'_{ij\ell m}$ through the relation

$$Q_{ij\ell m} = Q'_{ij\ell m} + Q_{Bjm} Q_{iB\ell} / (1 - Q_{BB}) \quad (4.35)$$

5. SOLUTION OF THE MULTIGROUP FLUX EQUATIONS

For each of the geometries we have discussed, the matrix equation satisfied by the P_0 and P_1 components of the flux can be written

$$\phi_{i\ell} = \sum_j V_j \sum_m Q_{ij\ell m} [S_{j\ell m} + \sum_{g'} \sum_{j'g'm} \phi_{j'g'm}] \quad (5.1)$$

The corresponding equation for the isotropic approximation is

$$\phi_{i\ell} = \sum_j V_j Q_{ij\ell} [S_{j\ell} + \sum_{g'} \sum_{j'g'} \phi_{j'g'}] \quad (5.2)$$

It is obvious that the methods employed in the solution of Equation 5.2 can easily be extended to the solution of Equation 5.1. A full discussion of the application of successive over-relaxation to the P_1 problem has been given by Harper (1967). The essential feature of this method is that the equations must be ordered so that the iteration matrix enjoys Property A which allows the estimation of an optimum over-relaxation parameter. In this section we will discuss the alternative block relaxation solution discussed for the isotropic problem by Doherty (1969).

We restrict ourselves to the P_1 approximation and note that the method which follows is clearly unsuitable for the solution of problems where more angular components are retained. In eigenvalue problems with no fixed source the term $S_{j\ell m}$ consists only of fissions which we shall assume to be isotropic.

Thus

$$S_{j\ell m} = (1/\lambda) \delta_{m0} \chi_g \sum_{g'} \nu \Sigma_{jg'}^F \phi_{jg'o} \quad (5.3)$$

where δ_{ij} is the Kronecker delta,

λ is the multiplication factor of the cell,

χ_g is the proportion of fission neutrons born in group g ,

and $\sum_{g'} \nu \Sigma_{jg'}^F \phi_{jg'o}$ is the fission neutron production rate.

If we write

$$T_{jg0} = (\chi_g / \lambda) \sum_{g'} \nu \Sigma_{jg'}^F \phi_{jg'o} + \sum_{g' \neq g} \Sigma_{jg'g0} \phi_{jg'o} \quad (5.4)$$

$$\text{and } T_{jg1} = \sum_{g' \neq g} \Sigma_{jg'g1} \phi_{jg'o} \quad (5.5)$$

then the set of Equations 5.1 for group g can be written

$$V_i \phi_{i\ell} = \sum_j V_j \{ Q_{ijg00} [T_{jg0} + \Sigma_{jgg0} \phi_{jg0}] + Q_{ijg01} [T_{jg1} + \Sigma_{jgg1} \phi_{jg1}] \} \quad (5.6)$$

$$V_i \phi_{i\ell} = \sum_j V_j \{ Q_{ijg10} [T_{jg0} + \Sigma_{jgg0} \phi_{jg0}] + Q_{ijg11} [T_{jg1} + \Sigma_{jgg1} \phi_{jg1}] \} \quad (5.7)$$

Concerning ourselves only with these equations for one group g , we define the following quantities.

$$\left. \begin{aligned} x_i &= V_i \phi_{i0} \\ x_{i+N} &= V_i \phi_{i0} \end{aligned} \right\} \quad (5.8)$$

$$\left. \begin{aligned} y_i &= V_i T_{ig0} \\ y_{i+N} &= V_i T_{ig1} \end{aligned} \right\} \quad (5.9)$$

$$\left. \begin{aligned} z_i &= \sum_{ig0} \\ z_{i+N} &= \sum_{ig1} \end{aligned} \right\} \quad (5.10)$$

Using these definitions Equations 5.6 and 5.7 can be recombined in the matrix form

$$Ix = Qy + Q(zx) \quad (5.11)$$

$$\text{Writing } Q(zx) = Rx \quad (5.12)$$

Equation 5.11 becomes

$$x = (I - R)^{-1} Qy \quad (5.13)$$

Standard matrix routines exist for the calculations of $(I - R)^{-1} Q$ which can be calculated for each group in turn and stored in place of the original Q . The solution process from this point on is precisely as given by Doherty (1969) for the isotropic problem. The general conclusions regarding the relative merits of this approach and SOR are much the same as for the isotropic calculation. Few-region, many-group problems are well suited to the block relaxation process while many-region, few-group problems can better be solved by SOR. The doubling of the dimension of the flux vector in each group enlarges the domain of applicability of SOR and reduces the domain of our method. However since it is likely that S_n codes will be used for large spatial problems in cylindrical geometry, and that the collision probability approach will find its niche in condensation calculations, we have adopted the block relaxation method.

6 GROUP CONDENSATION

As presaged in the previous section, a probable application of the anisotropic collision probability calculation is to provide suitable collapsing spectra for use in energy group condensation. A discussion of P_0 condensation procedures has been given by Doherty (1970). The expansion to P_1 fluxes allows us to condense the P_1 scattering matrix over its appropriate spectrum, thus avoiding difficulties in the condensation of the transport cross section.

Define the following quantities:

$\Sigma_{gg'0}$ = the P_0 scattering cross section from group g to group g'

$\Sigma_{gg'1}$ = the P_1 scattering cross section from group g to group g'

Σ_g^T = the total cross section in group g

Σ_g^{tr} = the transport cross section in group g

Σ_g^a = the absorption cross section in group g

ϕ_{g0} = the P_0 flux in group g

ϕ_{g1} = the P_1 flux in group g .

Suppose we wish to collapse the groups (indexed by g) to form a large group G . Then we proceed as follows:

$$\phi_{G0} = \text{Sum}_g \phi_{g0} \quad (6.1)$$

$$\phi_{G1} = \text{Sum}_g \phi_{g1} \quad (6.2)$$

$$\Sigma_G^a = \text{Sum}_g (\phi_{g0} \Sigma_g^a) / \phi_{G0} \quad (6.3)$$

Reaction rates involve only the scalar flux ϕ_{g0} which explains its appearance in Equation 6.3. The total cross section is similarly obtained

$$\Sigma_G^T = \text{Sum}_g (\phi_{g0} \Sigma_g^T) / \phi_{G0} \quad (6.4)$$

The scattering cross sections are averaged, each over its appropriate spectrum.

$$\Sigma_{GG'0} = \text{Sum}_g \phi_{g0} (\text{Sum}_{g'} \Sigma_{gg'0}) / \phi_{G0} \quad (6.5)$$

$$\Sigma_{GG'1} = \text{Sum}_g \phi_{g1} (\text{Sum}_{g'} \Sigma_{gg'1}) / \phi_{G1} \quad (6.6)$$

We come now to the transport cross section which poses our major problem in the isotropic case. By definition, the transport cross section for group g is

$$\Sigma_g^{tr} = \Sigma_g^T - \text{Sum}_{g'} \Sigma_{gg'1} \quad (6.7)$$

If we have available the P_1 spectrum ϕ_{g1} and the P_1 scattering matrix $\Sigma_{gg'1}$ then we could use the following definition of the condensed transport cross section:

$$\Sigma_G^{tr} = \Sigma_G^T - \text{Sum}_G \Sigma_{GG'1} \quad (6.8)$$

Where either the P_1 spectrum or the P_1 scattering matrix is unavailable we have in the past used the WIMS prescription (Askew et al. 1966):

$$\Sigma_G^{tr} = \Sigma_G^a + \phi_{G0} / [\text{Sum}_g \phi_{g0} / (\Sigma_g^{tr} - \Sigma_g^a)] \quad (6.9)$$

If we have performed a P_1 condensing calculation and are about to embark on a P_0 main transport calculation then we must decide between Equation 6.8 and Equation 6.9 for our method of calculating the transport cross section. We shall return to this point in the next section. However if the main transport calculation is to be P_1 then it is the total cross section of Equation 6.4 which is required and not the transport cross section. In this case the condensing procedure outlined above is a substantial improvement over that proposed by Harper (1967).

7. DISCUSSION

The theory of the preceding sections has been coded for the IBM 360/50 computer. In slab geometry the time spent in computing the collision probability matrix for the anisotropic case is 1.9 times that required for an isotropic problem with the same numbers of regions and groups. The corresponding factors for spherical and cylindrical geometries are 2.3 and 3.4 respectively. The large increase for cylindrical geometry is due to the need to evaluate three independent functions K_{i3} , K_{i4} , and K_{i5} in the anisotropic problem where in the isotropic problem only K_{i3} was required. The increases in slab and cylindrical geometries are not so dramatic because the anisotropic and isotropic problems both require the evaluation of the same number of exponentials.

The solution of the multigroup equations for the fluxes can be divided into a precomputation stage and an iteration stage. In the precomputation stage the matrix $(I - R)^{-1} Q$ is evaluated for each group. Since the dimension of the flux vector is doubled in the anisotropic problem the time for this

stage is increased by a factor of 8. In the iteration stage the operation is essentially the multiplication of a matrix by a vector so the increase is a factor of 4. The overall increase in time for the solution process therefore lies between 4 and 8, approaching the lower limit for many-group, few-region problems, and the upper limit for few-group, many-region problems.

This solution process is extremely stable from problem to problem and the time for solution is virtually independent of the geometry. That is to say, the same number of mesh regions with the same group structure will always take about the same time. Typical figures for an anisotropic problem are 0.8 minutes for a 69 group, 3 region problem and 0.6 minutes for a 16 group, 11 region problem. We may expect that the corresponding times for a solution process using SOR will be roughly comparable.

In contrast to the collision probability approach, the extension of the S_n method to the P_1 scattering problem is trivial, both in implementation and in the time penalty incurred by the inclusion of the additional term. The P_1 flux ϕ_{1g1} is obtained from the angular fluxes by a quadrature rule in exactly the same way as the scalar flux ϕ_{1g0} is already computed. The additional source into each angular direction resulting from the P_1 scattering term is easily computed, and the time involved in the computation of outscatters increases linearly with the order of anisotropy. The iteration strategy is unaffected by the presence of the P_1 component, and in most cases the rate of convergence should be the same as for the isotropic problem. Thus the overall increase in time for an S_n solution should be considerably less than a factor of 2.

These considerations severely restrict the class of problem for which an anisotropic collision probability solution should be contemplated. Isotropic collision probability calculations are normally performed for few-region, many-group problems where the collision probability calculation time is small and a good proportion of the total calculation time is taken up by the flux solution process. Even for these problems the inclusion of the P_1 term will increase the time by a factor of 4, against a maximum of 2 for the corresponding S_n solution. For many region problems the collision probability factor will approach 8 while the S_n factor is unchanged. Thus the rightful province of the anisotropic collision probability calculation is constrained to the group condensation type of problem with a minimal number of regions.

Group condensation using the fine group P_1 spectrum was discussed in the previous section. Even if it is intended to perform the main transport calculation in the P_0 approximation, we are not precluded from performing the condensation calculation in P_1 . This being the case, a choice must be made between the alternative forms of the transport cross section given in Equations 6.8 and 6.9. To shed some light on this problem we have examined a 0.5 cm radius, 3% enriched uranium rod surrounded by an annulus of water with a reflective outer boundary at radius 0.75 cm. The condensing calculation was performed in the P_1 approximation using 69 groups corresponding as closely as possible to those of the WIMS set (Askew et al. 1966).

The condensing calculation was performed with two regions; one in the fuel and the other in the water. An 18 group set of collapsed cross sections was prepared for the water and the fuel. Three different water cross sections were produced; a R_0 set computed using Equation 6.8, a P_0 set computed using Equation 6.9 and a P_1 set. The calculation was then repeated using the 18 group sets. The k -infinity results are shown in Table 1. The agreement between the 69 group and 18 group P_1 calculations shows that our collapsing procedure for the P_1 cross sections is adequate. The difference between the P_0 and P_1 calculations is small enough to assert that P_0 calculations will suffice for this type of system. Finally the difference between the two P_0 calculations is insignificant, despite some significant differences in the transport cross sections which are shown in Table 2. Group 18 is the same as the last group of the 69 group set so no condensation has taken place for this group.

In cell calculations the influence of the transport cross section on k -infinity results is usually small for several reasons. The main one is that the self scattering cross section for the group is always related to the total cross section (or transport cross section in the transport approximation) by the formula:

$$\text{self scatter} = \text{total} - \text{absorption} - \text{outscatter.}$$

This ensures that to first order, the absorption reaction rate for the material is independent of the value of the total cross section of the material. In small cells, where the spatial variation of the flux is also small, large errors in the transport cross section can be tolerated. The situation with regard to k effective calculations is not the same because errors in the transport cross section, and hence the diffusion coefficient, are reflected immediately in the estimate of leakage. For the cell we have been discussing where the leakage must account for 20 percent of the neutrons an error of 5 percent in D will amount to an error of 1 percent in k effective. It seems clear then, that in judging an approximation for the transport cross section in cell calculations, paramount importance must be attached to the effect on leakage of the approximation. We have therefore preferred to use Equation 6.9 which preserves the conventional method of collapsing diffusion coefficients.

From our experimentation with the Pressurised Water Reactor type of cell there seems little to be gained from the extra computation involved in the P_1 approximation. It is possible that in larger cells, such as those of pressure tube reactors, the use of the P_1 approximation may be marginally worth while. We cannot test this hypothesis at present because P_1 data for moderators other than H_2O are still in preparation. Comparative calculations will be made when the data are available.

We examined two spherical systems where the use of the transport approximation with P_0 scattering might be expected to give large errors in the estimate of k -effective. The first was a bare sphere, 18 cm in radius, containing a 5 percent by weight enriched UO_2 , H_2O mixture. The second system was the same, but surrounded by 30 cm of H_2O . These systems were run using the spherical collision probability routine discussed in Section 3 and also with the discrete ordinates code ANISN (Engle 1967). The results are presented in Table 3.

Firstly we note that the S_n code was run with 150 mesh intervals and the collision probability code with 24 regions. Ideally the number of mesh regions in the collision probability calculation should have been about 40 for the bare system and 100 for the reflected system. The flat flux assumption underlying collision probability theory leads to a significant overestimate of the leakage in bare spheres. The only way to avoid this error without building a more general flux shape into the theory is to increase the number of mesh intervals. Both the storage and run time requirements of collision probability calculations increase rapidly with the number of mesh intervals and so in general we prefer to use the S_n approach. The differences between the S_n and collision probability P_0 results are due entirely to the inadequate mesh representation used in the collision probability calculations. For the bare system where the mesh intervals are smaller in the collision probability code the agreement between the two methods is much improved.

Confining ourselves to the S_n results which are more reliable we see that for both the bare and reflected systems the P_1 estimate of k -effective is slightly less than 1 percent higher than the P_0 estimate. Obviously the difference between the two will depend on the system under study and on the group structure employed but this is the order of the effect. In these spheres the flux is highly anisotropic towards the outer boundary so the agreement is really quite good. In cell calculations where the same anisotropy of flux is not expected, the P_0 calculation should suffice.

The use of P_1 scattering in the collision probability calculations gives an increase of 1.4 percent for the reflected system. The difference from the S_n result lies in the error introduced by the approximation of Equation 3.14 and 3.15. For the smaller mesh intervals of the bare system the agreement is much better. It is worthwhile emphasising again at this point that only for slabs can the anisotropic collision probability result be considered exact. Both of the curved geometry routines contain a numerical approximation in the evaluation of the P_1 probabilities, in addition to the flat flux assumption common to all collision probability methods.

8. CONCLUSION

It appears that the collision probability methods developed here have little application outside their possible use in providing P_1 spectra for condensation. Systems where the P_1 approximation is required usually exhibit scalar flux gradients which are much better approximated in the S_n method of solution which consequently requires fewer mesh points. However the most compelling argument in favour of the S_n method is that the extension to P_1 or even higher orders of anisotropy can be accomplished with a modest increase in storage and computation time. Unfortunately the same cannot be said for the collision probability method.

The discrete integral transport approach of Carlvik (1966) offers some advantages over conventional collision probabilities in these geometries. The quantities calculated in the Carlvik scheme are not the mean fluxes over region as in collision probabilities but the fluxes at discrete points within the region. The discrete points are ordinates in a Gauss quadrature scheme in the manner suggested by Kobayashi and Nishihara (1964). Firstly if the same number of discrete points are present in the Carlvik scheme as there are regions in the corresponding collision probability calculation then the amount of computing time required is reduced to about 1/4 for the calculation of the transfer matrix. The solution time remains the same for the same size problem.

The other advantage inherent in Carlvik's scheme is that the extension to anisotropy is not plagued by approximations of the type displayed in Equation 4.20. The discrete space representation permits the evaluation of the higher l components of the transfer matrix with the same ease as the $l = 0$ components. In isotropic calculations the available evidence confirms the superiority of the Carlvik method. In anisotropic calculations the method suffers from the same disadvantage as collision probabilities in that the same increases apply to the various computing times as applied in the collision probability case. The S_n method retains its superiority.

9. REFERENCES

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TABLE 1
k-INFINITY RESULTS FOR PWR CELL

Run	k-infinity
69 group P_1	1.2637
18 group P_1	1.2637
18 group P_o , transport from Equation 6.8	1.2642
18 group P_c , transport from Equation 6.9	1.2642

TABLE 2
18 GROUP WATER TRANSPORT CROSS SECTIONS FOR PWR CELL

Group	Σ^{tr} from Equation 6.8	Σ^{tr} from Equation 6.9	% Difference
1	0.0769	0.0756	1.8
2	0.1106	0.1074	3.0
3	0.2130	0.2128	0.0
4	0.3335	0.3304	0.9
5	0.3972	0.3843	3.4
6	0.5003	0.4750	5.3
7	0.5289	0.5369	-1.5
8	0.5643	0.5633	0.2
9	0.5693	0.5694	0.0
10	0.5737	0.5737	0.0
11	0.5793	0.5795	0.0
12	0.5972	0.5903	1.2
13	0.5841	0.5969	-2.2
14	0.7509	0.7431	1.0
15	1.1719	1.1394	2.9
16	2.1172	2.0286	4.4
17	3.8245	3.7434	2.2
18	6.6154	6.6154	0.0

TABLE 3

k-EFFECTIVE RESULTS FOR SPHERICAL SYSTEMS

System	Calculation	Scattering Representation	No. Mesh Regions	k-effective
Reflected	S_n	F_0	150	1.0016
"	S_n	P_1	150	1.0108
"	C.P.	P_0	24	0.9686
"	C.P.	P_1	24	0.9830
Bare	S_n	F_0	150	0.8264
"	S_n	P_1	150	0.8344
"	C.P.	P_0	24	0.8129
"	C.P.	P_1	24	0.8292

