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THREE-DIMENSIONAL LMFBR SHIELDING
DESIGN AND ANALYSIS CODE

Quarterly Progress Report

Claude G. Poncelet and James A. Bucholz

Carnegie-Mellon University
Pittsburgh, Pennsylvania 15213

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ABSTRACT

This progress report describes the development of a design-oriented three-dimensional transport method for shielding calculations. The method, as originally suggested by Wagner, uses 14 angular directions, or rays, within an array of uniform cubical mesh blocks, with the rays continuous at block interfaces and passing through the centers of the blocks. The integral transport equation is solved analytically along the rays within a block, with outgoing rays becoming incoming rays for adjacent blocks. Extensions of the method are described to include full anisotropic scattering based on integrated ray-to-ray scattering probabilities, variable mesh capability, and generalized boundary conditions including vacuum, reflection with arbitrary albedo, periodic, and specified source. A computer code, TRANS3, has been developed to incorporate the method and its various extensions, and the program logic is described. The code has multigroup capability and will perform fixed source or eigenvalue calculations. Appropriate use of the reflective boundary condition permits use of the code in one- or two-dimensional geometries. The selection of efficient spatial mesh sweeping algorithms and of efficient iterative schemes in the solution of the ray equations is summarized.

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PROGRAM DESCRIPTION

The objective of this program is the development and evaluation of a rapid three-dimensional industrial design tool for shielding calculations. The program consists of the following technical tasks.

TASK 1 - Method Development

The aim of this task is to extend the three-dimensional 14-ray Direct-Coupled Ray (DCR) neutron transport method, originally proposed by Wagner, to include anisotropic scattering, generalized boundary conditions, and variable spatial mesh capability. An extension to a 26-ray formalism is to be outlined, with implementation conditional on evaluation of the adequacy of the 14-ray model.

TASK 2 - Code Development

Under this task a multigroup, three-dimensional computer program is to be developed to incorporate the basic DCR method with the various extensions developed under Task 1.

TASK 3 - Evaluation of Numerical Algorithms

The aim of this task is to evaluate and select numerical and coding algorithms, such as spatial mesh sweeping, iterative, and dynamic storage allocation schemes for best overall computational efficiency.

TASK 4 - Method and Code Verification and Evaluation

Under this task, the method and code developed under Tasks 1, 2 and 3 are to be tested and evaluated for LMFBR shielding applications. Calculations are to include specific benchmark calculations for code and method verification, and scoping calculations to investigate space-angle coupling characteristics of the method, spatial mesh block size requirements, and speed and accuracy characteristics.

1.0 TASK 1 - METHOD DEVELOPMENT

1.1 The Basic Direct Coupled Ray Method

The method proposed herein for LMFBR shielding design and analysis will be denoted the Direct-Coupled Ray (DCR) method. The computational approach was originally suggested by Wagner, et.al.(1) and a version implemented in the 3DT code for the safety analysis of the thermionic critical experiment at Gulf General Atomic(2,3).

In its simplest form, the DCR method considers a three-dimensional assembly in the form of a rectangular parallelepiped which is composed of a finite number of cubical blocks. Each block or any arbitrary combination of blocks may represent a separate spatial region of given composition. Within each block are defined the 14 angular flux components shown in Fig. 1. Constant mesh spacing in each spatial direction allows the choice of angular directions which are continuous through block boundaries and which pass through the centers of neighboring blocks thereby avoiding the time consuming interpolation between neighboring cell angular fluxes.

It is assumed that the neutron flux can be described in terms of 14 angular flux components $\phi_{i,j,k,\ell}(s_\ell)$ $\ell = 1, \dots, 6$ and $\phi_{i,j,k,m}(s_m)$ $m = 1, \dots, 8$ as shown in Fig. 1 where i, j, k are the spatial indices of the block and s_ℓ or s_m denote the path length along the corresponding ray. The Boltzman transport equation in rectangular geometry may be written as:

$$\mu \frac{\partial \phi}{\partial x} + \eta \frac{\partial \phi}{\partial y} + \xi \frac{\partial \phi}{\partial z} + \Sigma_T \phi = S \quad (1)$$

where $\mu = \frac{\partial x}{\partial s}$, $\eta = \frac{\partial y}{\partial s}$, $\xi = \frac{\partial z}{\partial s}$ are the direction cosines of a given ray.

Illustrating with only the normal components, this may be written as:

$\phi_{i,j,k,\ell}$ - Outgoing Normal Components

$\phi_{i,j,k,m}$ - Outgoing Diagonal Components

ψ_ℓ, ψ_m - Incoming Flux Components

Figure 1
Angular Directions of the Basic DCR Method

$$\frac{d\phi_{i,j,k,\ell}(s_\ell)}{ds_\ell} + \Sigma_T \phi_{i,j,k,\ell}(s_\ell) = S_{i,j,k,\ell}(s_\ell) \quad (2)$$

where $S_{i,j,k,\ell}(s_\ell)$ represents the intrinsic and external sources along the ray. Assuming that the source term $S_{i,j,k,\ell}(s_\ell)$ is constant along the path length s_ℓ within block i,j,k as is done with Discrete Ordinates methods, the Boltzman equation may be integrated analytically along any given ray. For a region characterized by isotropic, or transport-corrected isotropic, scattering, the resulting multigroup ray equations can be expressed as:

$$\begin{aligned} \phi_\ell^g &= \Gamma_\ell^g \psi_{\ell+3}^g + \Delta_{F^g}^g & \ell &= 1, 2, 3 \\ \phi_\ell^g &= \Gamma_\ell^g \psi_{\ell-3}^g + \Delta_{F^g}^g & \ell &= 4, 5, 6 \\ \phi_m^g &= \gamma_m^g \psi_{m+4}^g + \delta_D^g & m &= 1, 2, 3, 4 \\ \phi_m^g &= \gamma_m^g \psi_{m-4}^g + \delta_D^g & m &= 5, 6, 7, 8 \end{aligned} \quad (3)$$

where ϕ_ℓ^g and ϕ_m^g are the outgoing angular flux components, ψ_ℓ^g and ψ_m^g are the incoming angular flux components, and superscript g denotes the energy group number. The isotropic source term F^g is defined in Eq. (A17) of Appendix I. The source term has an intrinsic dependence on the scalar flux and, if neutron balance is to be preserved, this will depend on the outgoing angular flux components ϕ_ℓ^g and ϕ_m^g . The parameters Γ_ℓ^g , γ_m^g , Δ^g and δ^g are block attenuation and build-up parameters, and are defined by Eqs. (A1-A5) in Appendix I.

The scalar flux ϕ^g is defined by setting

$$\phi^g = \sum_{\ell=1}^6 W_\ell \bar{\phi}_\ell^g + \sum_{m=1}^8 W_m \bar{\phi}_m^g \quad (4)$$

where $\bar{\phi}_\ell^g$ and $\bar{\phi}_m^g$ are integral averages defined by

$$\bar{\phi}_\ell^g = \frac{1}{h} \int_0^h \phi_\ell^g(s_\ell) ds_\ell$$

$$\bar{\phi}_m^g = \frac{1}{h\sqrt{3}} \int_0^{h\sqrt{3}} \phi_m^g(s_m) ds_m$$
(5)

where $\phi_\ell^g(s_\ell)$ and $\phi_m^g(s_m)$ are the analytic solutions to the integral transport equation along the various rays within a block, and h is the linear size of the cube. In Eq. (4) it is convenient to define equal weights $W_\ell = W_m = \frac{1}{14}$. The resulting expression for the scalar flux contains incoming and outgoing angular flux components. The outgoing components may be eliminated by making use of the ray equations (3) with the source term F^g defined by Eq. (A17). Collecting terms in ϕ^g , the result is Eq. (A13) of Appendix I. This equation, along with the ray equations (3) are the basic equations of the DCR method. The equations are solved iteratively, as indicated in equations (A19) and (A20) of Appendix I, where n denotes the inner iteration number.

As may be seen from the ray equations and Fig. 1, the outgoing angular flux component on any face (or corner) of a block is written directly in terms of the corresponding incoming angular component on the opposite face (or corner). While passing through a block (i,j,k) which is completely in the interior of an assembly, the incoming components $\psi^{g,n-1}(i,j,k)$ and $\psi_m^{g,n-1}(i,j,k)$ are collected as outgoing components from the adjacent blocks, as noted in equation (A12) of Appendix I. Otherwise, each point at

which a ray penetrates the external surface of the assembly may be given its own boundary condition for each energy group. The incoming angular flux components are held fixed momentarily as one calculates the scalar flux $\phi^{g,n}(i,j,k)$ and the new outgoing angular flux components $\phi_l^{g,n}$ and $\phi_m^{g,n}$ for that block from the ray equations. Note that in the case of isotropic within-group scattering, the ray equations for a given block are decoupled and represent 14 algebraic equations. Applying the appropriate boundary conditions, these equations are solved in one block after another as one marches through the assembly, reversing the direction of the march during each inner iteration.

Convergence of the inner spatial iterations is accelerated by scaling. A group scaling factor f^g is determined from the condition that the overall neutron balance for the whole assembly is fulfilled within each energy group. One has

$$f^g = \frac{Q^g}{A^g + L^g} \quad (6)$$

where Q^g is the total group source in the assembly, A^g is the total group removal rate via absorption or out-scattering for the whole assembly, and L^g is the net group leakage out through the external surface of the assembly. These terms are more fully defined in equations (A21), (A22) and (A23) of Appendix I. These equations are obtained by writing the neutron balance for a particular block and summing over all blocks of the assembly. The group scaling factor f^g is used to adjust all scalar and angular group fluxes before starting the next inner spatial iteration.

The following sections under Task 1 describe the extension of the basic

DCR method to incorporate full anisotropic scattering, arbitrary boundary conditions, and variable mesh capability.

1.2 Anisotropic Scattering Treatment

The formulation of a full anisotropic scattering model requires a clear understanding of the ray-to-ray scattering probabilities. With the fourteen angular directions previously defined, there are seven possible scattering angles (0° , 54.7° , 70.5° , 90° , 109.5° , 125.3° , 180°). Knowledge of the differential scattering cross sections $\Sigma_s^{g' \rightarrow g}(\mu_i)$, where μ_i , $i=1, \dots, 7$ is the cosine of the scattering angle, is insufficient to correctly define the various probabilities in an integral sense. As shown in Fig. 2, a ray entering normal to the face of a block has

- 1 exit channel at 0°
- 4 exit channels at 54.7°
- 4 exit channels at 90°
- 4 exit channels at 125.3°
- 1 exit channel at 180°

On the other hand, as shown in Fig. 3, a ray entering through a corner of a block has

- 1 exit channel at 0°
- 3 exit channels at 54.7°
- 3 exit channels at 70.5°
- 3 exit channels at 109.5°
- 3 exit channels at 125.3°
- 1 exit channel at 180°

Hence, care must be established in associating solid angles with the

Figure 2
Ray-to-Ray Scattering Angles for
an Incoming Normal Ray

Figure 3
Ray-to-Ray Scattering Angles for an Incoming Diagonal Ray

scattering probabilities. For example, a different range of scattering angle μ must be used to calculate the scattering probability about 54.7° in the two cases above.

Given that a ray enters from the right, as depicted in Fig. 4, and associating a solid angle of $4\pi/14$ with each ray, one can establish the proper ranges of μ required in defining integral scattering probabilities with the use of geometrical arguments. In this fashion nine partial ray-to-ray scattering cross sections $\Sigma_S^i(g' \rightarrow g)$, $i=1, \dots, 9$ may be defined, as detailed in Eq. (A8) of Appendix I. These scattering cross sections have the form

$$\Sigma_g^i(g' \rightarrow g) = \frac{2\pi}{N} \int_a^b \Sigma_S^{g' \rightarrow g}(\mu) d\mu \quad (7)$$

where a and b take on the values $(-1, -6/7, -3/7, 0, 3/7, 6/7, 1)$, and N takes on the values $(1, 3, 4)$. For reference, the total scattering cross section is given by

$$\Sigma_S^{g' \rightarrow g} = 2\pi \int_{-1}^1 \Sigma_S^{g' \rightarrow g}(\mu) d\mu \quad (8)$$

Anisotropic scattering of any order may be included by integrating the polynomials for which the group to group Legendre coefficients are given. These coefficients may be supplied in either ANISN or DTF-IV format.

The full anisotropic scattering source for any given ray is obtained by multiplying the block-averaged angular fluxes $\bar{\psi}_\ell^{g,n-1} = \bar{\phi}_{\ell \pm 3}^{g,n}$, $\bar{\psi}_m^{g,n-1} = \bar{\phi}_{m \pm 4}^{g,n}$

Figure 4

Solid Angles Associated with Ray-to-Ray Scattering Probabilities

by the appropriate partial scattering cross sections and summing over all rays. The anisotropic scattering source for the outgoing angular flux component $\phi_1^{g,n}$, for example, is given by

$$\begin{aligned}
 S_1^{g,n} = \Delta^g \sum_{g'=1}^G \left\{ \Sigma_S^1(g' \rightarrow g) \bar{\psi}_1^{g',n-1} + \Sigma_S^2(g' \rightarrow g) \left[\bar{\psi}_2^{g',n-1} + \bar{\psi}_4^{g',n-1} \right. \right. \\
 + \left. \bar{\psi}_5^{g',n-1} + \bar{\psi}_7^{g',n-1} \right] + \Sigma_S^5(g' \rightarrow g) \left[\bar{\psi}_2^{g',n-1} + \bar{\psi}_3^{g',n-1} \right. \\
 + \left. \bar{\psi}_5^{g',n-1} + \bar{\psi}_6^{g',n-1} \right] + \Sigma_S^8(g' \rightarrow g) \left[\bar{\psi}_1^{g',n-1} + \bar{\psi}_3^{g',n-1} \right. \\
 \left. \left. + \bar{\psi}_6^{g',n-1} + \bar{\psi}_8^{g',n-1} \right] + \Sigma_S^9(g' \rightarrow g) \bar{\psi}_1^{g',n-1} \right\} \quad (9)
 \end{aligned}$$

where Δ^g is defined in Eq. (A4) of Appendix I. The anisotropic scattering source terms for the remaining rays can be readily defined in a similar fashion.

With an anisotropic scattering source, the DCR ray equations for a given block represent a set of 14 coupled, linear equations. This may be seen by noting that the source terms described above contain the block-averaged angular flux components, as defined by Eq. (5) which, as shown in Eq. (A14) of Appendix I, can be written in terms of incoming and outgoing angular flux components along a given ray. The full anisotropic ray equations can be put in the form

$$A \phi^{g,n} = S^{g,n-1} \quad (10)$$

where $\phi^{g,n}$ is a column vector of the outgoing angular flux components, $S^{g,n-1}$ is a source column vector which includes incoming angular flux components and the scattering and fixed source terms, and A is a full 14×14 matrix whose elements are functions of the total removal and in-scattering cross sections, and of the mesh size.

In contrast to the case of isotropic scattering, the outgoing angular flux components cannot be eliminated a priori from the equation for the scalar flux, such that the scalar flux $\phi^{g,n}$ must be calculated directly from Eq. (4) after the system of Eq. (10) has been solved. The iterative scheme utilized in the solution of Eq. (10) will be further discussed in Section 3.0.

In the case of P_1 scattering, the present formulation does differ somewhat from the original work done by Wagner(1). Indeed, if the partial scattering cross sections $\Sigma_s^i(g' \rightarrow g)$ are defined in a discrete sense, only at the seven possible scattering angles as in Eq. (A9) of Appendix I, rather than in an integral sense as described herein, the resulting P_1 ray equations reduce identically to those of Wagner.

As with isotropic scattering, convergence of the inner spatial iterations is accelerated by scaling. The group scaling factor is given by Eq. (6), where it can be readily shown that Q^g , A^g and L^g are again calculated from Eqs. (A21), (A22) and (A23) of Appendix I.

1.3 Generalized Boundary Conditions

Arbitrary boundary conditions may be assigned at each spatial point at which a ray penetrates the surface of the assembly, for each energy group. Generalized boundary conditions may be derived to include vacuum, reflection with arbitrary albedo, periodic, and specified source conditions. For a ray ψ_{ℓ}^g entering the assembly normal to the surface, these conditions take the general form

$$\text{Vacuum} \quad \psi_{\ell}^g = 0 \quad (11)$$

$$\text{Reflection} \quad \psi_{\ell}^g = \alpha_{\ell}^g \phi_{\ell}^g \quad (12)$$

$$\text{Periodic} \quad \psi_{\ell}^g(i,j,k) = \phi_{\ell \pm 3}^g(i',j',k') \quad (13)$$

$$\text{Specified Source} \quad \psi_{\ell}^g = S_{\ell}^g \quad (14)$$

where α_{ℓ}^g is an arbitrary albedo, S_{ℓ}^g is a known, specified angular source component, and $(i,j,k), (i',j',k')$ denote mesh blocks on opposite sides of the assembly.

In developing the boundary condition algorithms for a three-dimensional assembly, as many as sixty-two (62) classes of rays penetrating the surface of the assembly must be considered. Development of the required algorithms is, however, a straightforward matter, and the specific equations for the four general boundary conditions noted above and all classes of incoming rays will not be reproduced here.

The use of the reflection boundary condition with unity albedo (perfect reflection) on appropriate surfaces of the assembly permits the computation of flux distributions in essentially one- or two-dimensional geometries. This capability is a particularly useful one in that it allows the analysis of a shielding configuration in one-, two-, or three-dimensions with the use of the same basic computational algorithm.

1.4 Development of a Variable Mesh Capability

A disadvantage of the basic Direct Coupled Ray method is the limitation to a uniform, cubic mesh throughout the assembly. Actually, the original work by Wagner(1) allows for non-cubic blocks with the angular directions chosen so as to pass through the corners of a block. Since in this case all blocks had the same dimensions, the essential property of the DCR method (i.e., the outgoing rays of one block become the incoming rays of the adjoining blocks and pass through the center of the adjoining blocks) was preserved. Because of the uniform mesh dimensions, however, the flexibility to describe many problems was not available and the more efficient use of smaller mesh size only in localized areas of interest was not provided for. A variable mesh capability, able to treat thin or non-regular regions is of interest in LMFBR shielding analysis.

Several concepts were examined in the development of a variable mesh capability. Very briefly, the following concepts were considered:

- (a) The Ray Splitting Technique. Illustrating this approach in one dimension with the normal components only, a given ray travelling to the right from a larger to a smaller mesh size

may be split into two or more equal components, while a given set of rays travelling from a smaller mesh to a larger mesh may be summed to obtain the resultant. The same may be done with all angular components. In this way both neutron balance

and neutron direction can be preserved. The major drawback of this approach is related to programming considerations because of the necessity to permit an arbitrary number, shape and location of zones of particular mesh size within a three-dimensional assembly.

- (b) Angular Interpolation Scheme. This scheme, based on the original approach of Wagner, ties the angular directions to the corners of a block while introducing a variable mesh. The principal difficulty is that at an interface where the mesh size changes, the diagonal rays are misaligned; i.e., they no longer are directly coupled and some interpolative scheme in angular (θ, ϕ) space is required.

Recall that one of the advantages of the DCR method is that the time-consuming interpolation between neighboring block angular fluxes can be avoided. An additional limitation is that in certain regions such as regions immediately adjacent to thin streaming paths, the angular flux $\psi(\underline{r}, \theta, \phi)$ may be a very sensitive function of θ and ϕ , leading to potentially large uncertainties in the angular interpolation. Lastly, it should be noted that these problems are not mitigated as the mesh size is further reduced.

(c) Spatial Interpolation Scheme. This scheme retains the fourteen angular directions defined by the faces and corners of a perfect cube and uses this quadrature even in non-cubic blocks. The result is that there is a spatial misalignment of the diagonal rays as one goes from a larger to a smaller mesh, and at the interface between any set of non-cubic blocks. This approach is less restrictive than

the previous method in that by reducing the mesh size, the spatial misalignment is mitigated. As with all S_N methods, the nominal mesh size should be chosen small enough that the angular flux in a given direction does not vary drastically over one or two mesh spaces. This is the scheme that has been selected for incorporation into the methodology.

Since a uniform cubical mesh is a basic feature of the DCR method, any variable mesh algorithm involves some approximations and care must be exercised in the use of such algorithm. Indeed relative accuracy requirements and computing costs must be considered in opting either for the use of a finer uniform cubical mesh, or for the use of the variable mesh algorithm.

In connection with the application of the variable mesh algorithm based on the spatial interpolation scheme, several characteristics of the scheme must be noted. First, the scheme is reasonably well adapted to accommodate

various irregular zones within an assembly that are either too large or too short to fit into an integer number of standard cubic meshes. However, a long series of all thin (or all thick) non-cubic blocks back-to-back should probably be avoided, since such an arrangement could compound the ray misalignment problem referred to earlier. If a large number of non-standard meshes is required, alternating oversized and undersized blocks may be advisable in order to mitigate the problem. In this situation, it may also be advisable to consider reducing the size of the standard cubic mesh.

Secondly, as the block shape is made to deviate farther and farther from a perfect cube, the incoming angular flux components to be used with the ray equations may best be described by angular components other than those on the opposite diagonals of that same block, as is the case for cubic blocks. The spatial interpolation scheme retains the 14 angular directions defined by the corners and faces of a perfect cube and uses this quadrature even in non-cubic blocks as shown in Fig. 5. Translating the outgoing components to the corners of the non-cubic block while maintaining the angular direction of the rays as shown in Fig. 6, it becomes apparent that the best incoming angular components for use with the ray equations are impingent somewhere on the largest face of the block rather than at the corners. Referring to Fig. 6, it becomes clear that as h_y is reduced still further, $\psi_6(i,j,k)$ will move closer to the upper left-hand corner and will have a numerical value closer to $\phi_2(i,j-1,k)$ than $\phi_2(i+1,j-1,k-1)$. Of course, with proper mesh size selection, this difference will be relatively small, and $\phi_2(i+1,j-1,k-1)$ may be assumed to act over the entire surface as is the case for cubic blocks. If the point (X_6, Z_6) is associated with the incoming component ψ_6 , a linear spatial interpolation of the form

Figure 5
Angular Directions Used in a
Non-Cubic Mesh Block

Figure 6
Three-Dimensional Ray Offset
in Variable Mesh Model

$$\begin{aligned}
\psi_6 = & \phi_2(i, j-1, k-1) + [\phi_2(i+1, j-1, k-1) - \phi_2(i, j-1, k-1)] \left(\frac{x_6}{h_x} \right) \\
& + [\phi_2(i, j-1, k) - \phi_2(i, j-1, k-1)] \left(\frac{z_6}{h_z} \right) \\
& + [\phi_2(i, j-1, k-1) + \phi_2(i+1, j-1, k) - \phi_2(i+1, j-1, k-1) \\
& - \phi_2(i, j-1, k)] \left(\frac{x_6}{h_x} \right) \left(\frac{z_6}{h_z} \right)
\end{aligned} \tag{15}$$

could be used. Such a correction may be helpful in relieving misalignment problems when large, flat regions are encountered or when one has a series of all thin (or all thick) non-cubic blocks back-to-back.

As discussed in Section 1.1, one associates with each ray an angular range or quadrature weight. For symmetry reasons the weights w_m for the diagonal components are equal for all directions. For the normal weights w_ℓ , symmetry requires that $w_\ell = w_{\ell+3}$ $\ell=1,2,3$. A further restriction on the normal weights may be derived from the requirement that the average square cosine with respect to all three spatial directions must be equal to 1/3 (i.e. the diffusion theory condition). This leads, for uniform cubic blocks to equal weights in all directions. When the shape of the block has been distorted from that of a perfect cube, since the angular directions remain fixed in space, one still has $\cos \theta = \frac{1}{\sqrt{3}}$ where θ is the angle between a diagonal ray and the x, y or z axes. Hence, with $w_m = w$

$$\begin{aligned}
\overline{\mu^2} &= 2w_1 + 8w \left(\frac{1}{\sqrt{3}} \right)^2 = \frac{1}{3} \\
\overline{\eta^2} &= 2w_2 + 8w \left(\frac{1}{\sqrt{3}} \right)^2 = \frac{1}{3} \\
\overline{\xi^2} &= 2w_3 + 8w \left(\frac{1}{\sqrt{3}} \right)^2 = \frac{1}{3}
\end{aligned} \tag{16}$$

From equation (16),

$$W_{\ell} = \frac{1}{6} (1-8W) \quad \ell=1,2,3 \quad (17)$$

and therefore the normal weights must be equal in all directions. Note that in Wagner's original work(1), the weights W_{ℓ} could differ because the angular directions were dependent upon the shape of the region. Defining a free parameter

$$\alpha = \frac{\frac{8W}{6}}{\sum_{\ell=1}^6 W_{\ell}} = \frac{4}{3} \quad (18)$$

and noting that one must have

$$\sum_{\ell=1}^6 W_{\ell} + 8W = 1 \quad (19)$$

yields

$$W_{\ell} = W = 1/14 \quad (20)$$

Allowing for different mesh sizes in the principal directions and noting that the track length through a non-cubic block along any diagonal ray is now given by

$$h_{DP} = \min \{h_x\sqrt{3}, h_y\sqrt{3}, h_z\sqrt{3}\} \quad (21)$$

one can derive the ray equations and the equation for the scalar flux in exactly the same fashion as described previously for isotropic or full anisotropic scattering.

The solution method for an assembly containing non-cubic blocks will remain essentially the same as before. The only exception is with regard to the calculation and application of the group scaling factor. Whereas previously there was a single group scaling factor f^g for the entire assembly, it is now necessary to divide the assembly into a number of

macroregions and define a group scaling factor f_M^g for each macroregion:

$$f_M^g = \frac{Q_M^g}{A_M^g + L_M^g} \quad (22)$$

where the terms Q_M^g , A_M^g and L_M^g are still calculated using equations (A21), (A22) and (A23) of Appendix I except that the summations appearing in Eq. (A23) should be replaced with summations over only those blocks (i,j,k) which are elements of the given macroregion M, and the summations appearing in Eq. (A21) should be taken over those normal and angular rays which penetrate the outside surface of the given macroregion M, including those on the

interior of the assembly. Formally, a macroregion is defined here as a rectangular parallelepiped composed of blocks of only one size and shape. The group scaling factors f_M^g are then used to adjust all scalar and angular group fluxes in their respective macroregions before starting the next inner spatial iteration.

Rigorously correct use of an acceleration scheme would require the definition and application of an individual group scaling factor f_M^g for each macroregion as defined above. Use of such multiple group scaling factors has been made in other computer codes. The use of any acceleration scheme, however, should be optional and should not affect the final result. Since complete cancellation of the normal components will always occur at the boundaries between macroregions and partial cancellation of the angular components will still occur at these boundaries, and since after the solution is reasonably well converged the appropriate scalar flux equation together with the discrete ordinate ray equations will maintain neutron balance within each of the individual blocks it has been found computationally expedient to use a single group scaling factor f^g for the entire assembly to accelerate towards a nearly correct solution, and then set $f^g = 1.0$ (i.e. stop using an acceleration scheme) during the last few iterations while the fluxes fine tune to the true solution.

It should be noted here that, although voids can be incorporated directly in the DCR formulation, and large voided regions can be represented adequately, streaming in long thin voided regions cannot be adequately represented by any of the variable mesh schemes discussed herein. This limitation, which is characteristic of all relatively low order discrete ordinates methods, arises because neutrons (or photons) originating at the

face of the void and streaming through the void at shallow angles are not properly accounted for. Because of the importance of streaming in long thin regions in shielding analyses, a special void streaming treatment has been developed for incorporation into the DCR method, and is discussed in the next section.

1.5 Special Treatment of Void Streaming

Within the context of the 14 ray model, integral transport in a vacuous region is described exactly by the ray equations. However, all surface sources are represented by a finite number of monodirectional rays, and there are some questions as to the adequacy of using only 14 rays to describe the transport within a void. Neutrons or photons entering an open-ended void at some shallow angle do have a certain probability of escaping out through the void which is not fully accounted for in the DCR model. Likewise, neutrons streaming up (or down) through the void at some slightly off-vertical angle do have a certain probability of entering the media, which is likewise not properly accounted for by the DCR model.

Although the first effect leads to an underestimate of void streaming, while the second effect leads to an overestimate of void streaming, thus causing some cancellation of errors, an attempt has been made to incorporate a special treatment of void streaming within the DCR model, because of the importance of such phenomena in shielding analyses.

The treatment of internal cavities and streaming paths proposed herein uses a line-of-sight method similar to that of Vossebrecker(4) but which is compatible with the 14 ray, three-dimensional DCR method. At the surface of each mesh element which is exposed to a voided region, a smooth continuous angular distribution $F_s(\theta, \phi)$ can be constructed which is a fit to the outgoing angular components at the surface of the element. With the proper definition

of solid angles, or lines of sight, the contributions of each surface element to the incoming angular components on surface elements on opposite faces of the voided region can be evaluated.

Referring to Fig. 1, it is seen that the surface angular distribution $F_s(\theta, \phi)$ should reproduce the five outgoing angular components defined on the given surface, and should approach the normal outgoing angular components on the four surfaces adjacent to the surface at hand, at the periphery of the hemisphere ($0 \leq \theta \leq \frac{\pi}{2}$, $0 \leq \phi \leq 2\pi$). A convenient fitting function is the even set of spherical harmonics functions, $Y_{2n-2}^m(\theta, \phi)$, defined by

$$Y_k^m(\theta, \phi) = \sqrt{\frac{2k+1}{4\pi} \frac{(k-m)!}{(k+m)!}} P_k^m(\cos \theta) [\cos m\phi + i \sin m\phi],$$

$$k \leq m \leq k \quad (23)$$

This set is complete and orthogonal over the hemisphere. With nine angular components known over the hemisphere, a unique surface distribution $F_s(\theta, \phi)$ can be generated as

$$F_s(\theta, \phi) = \sum_{n=1}^3 \sum_{m=-(2n-2)}^{(2n-2)} A_{n,m} Y_{2n-2}^m(\theta, \phi) \quad (24)$$

where $A_{n,m}$ are mixing coefficients. Note that for any real function such as $F_s(\theta, \phi)$, one must have $A_{n,-m} = A_{n,m}$, leaving nine independent mixing coefficients $A_{n,m}$ to be determined from the known angular flux components f_i , $i=1, \dots, 9$. Inverting the coefficient matrix, each $A_{n,m}$, and hence

$F_s(\theta, \phi)$, may be written as a linear combination of the angular flux components f_i , where the combination coefficients depend only on the 14 angular directions defined in Fig. 1, and are therefore constants for any given voided region. By proper integration of the function $F_s(\theta, \phi)$ over the solid angles which define the appropriate lines of sight, the incoming angular flux components on other surface elements of the voided region can be calculated as a sum of linear combinations of the outgoing angular flux components from surface elements on opposite faces of the void region. For a given surface element of the voided region, this may be written as

$$\underline{\psi}^g = V \underline{\phi}^g \quad (25)$$

where $\underline{\psi}^g$ contains the incoming angular flux components on a surface element, $\underline{\phi}^g$ contains the outgoing angular flux components on all the other surface elements on opposite faces of the void, and V is a void streaming matrix. From the discussion above it can be seen that the void streaming matrix depends only on geometry, and need be calculated only once for each surface element of the voided region. For practical purposes, it may be necessary and adequate to approximate the streaming matrix V to limit the calculation of surface element to surface element coupling.

The above treatment of void streaming within the context of the 14 ray DCR method properly preserves the geometric effects of void streaming, and is limited only by the relative accuracy of the fitted functions $F_s(\theta, \phi)$ in representing the angular flux distribution on the void surfaces. Two important advantages of the method are that voids of arbitrary size, shape and location can be modelled in three dimensions, and that the treatment of void streaming is consistent with the logic of the mesh sweeping algorithm of the basic ray equations.

1.6 Extension to 26-Ray Formalism

The essence of the DCR method, conceptually stated, is that constant mesh spacing in each spatial direction allows the choice of angular directions which are continuous through block boundaries and which pass through the centers of neighboring blocks. The 14 ray scheme, as originally proposed by Wagner(1), has been shown in Fig. 1. Kinnebrack(5) has described a 24 ray scheme in rectangular geometry, by introducing a coupling to second nearest neighbors. An extension to 26 rays in rectangular geometry would, however, be possible while maintaining all of the features of the DCR method.

The 26 ray scheme would include the 14 rays shown in Fig. 1 plus 12 additional rays extending from the center of the mesh block to the midpoint of each edge as shown in Fig. 7. The use of the 26 ray scheme would improve space-angle coupling but would increase core storage requirements and machine running time. However, its use may also permit the use of larger spatial mesh size, thus implying some trade-off.

For the case of isotropic, or transport-corrected, isotropic scattering, the extension to a 26 ray scheme is straightforward, with appropriate attenuation and build-up factors defined for the additional rays in the ray equations. For the case of full anisotropic scattering, not only would a larger number of ray-to-ray scattering angles be introduced, but several new sets of partial scattering cross sections would also have to be defined so as to accurately describe the probabilities. As noted in Section 1.2, the number of partial scattering cross sections that has to be defined is greater than the number of ray-to-ray scattering angles. The anisotropic, 26 ray equations can again be written in the form of Eq. (10), where now A is a 26×26 matrix. With the 26 ray scheme, there are 36 new classes of rays penetrating the outer surface of a three-dimensional assembly for which

Figure 7
Additional Angular Directions Used in
the 26 Ray Scheme

specific boundary condition algorithms have to be specified for each of the four general boundary conditions discussed in Section 1.3.

The desirability and need for a 26 ray version of the DCR method obviously depends on the relative adequacy, from both an accuracy and computer running time point of view, of the 14 ray version in the analysis of shielding configurations. Since space-angle coupling, and therefore the treatment of particle transport, is improved in the 14 ray DCR method by reducing the spatial mesh size, and since the 26 ray method would require additional computer storage and computation time, it does not follow a priori that a 26 ray calculation with larger mesh blocks would be preferable to a 14 ray calculation with smaller mesh blocks.

Because of these considerations, and in view of the additional effort required in programming the 26 ray method, it has been concluded that the 14 ray method, with its various extensions described in earlier sections, should be fully investigated and evaluated in shielding analyses, before the need for programming the 26 ray version is established.

2.0 TASK 2 - CODE DEVELOPMENT

2.1 The TRANS3 Code

The basic DCR method, along with the extensions to include full anisotropic scattering capability, generalized boundary conditions, and variable mesh capability, has been programmed and the computer code has been labeled TRANS3. Programming has been done in standard Fortran IV, and the code implemented on the Carnegie-Mellon University IBM-360(TSS)/67 and UNIVAC-1108 computers.

A flow diagram showing the computational logic of the code is included in Appendix II. The code has multigroup capability and will solve either fixed source or eigenvalue problems. Equation numbers on the flow diagram refer to working equations listed in Appendix I. Upon reading the input data, blockwise and groupwise parameters are computed; the ray equations are solved by sweeping through the mesh, and the scalar flux is computed. The group scaling factors are computed, and the ray equations are solved iteratively to convergence.

Detailed descriptions of subroutine functions will be provided in a later report. The following subsections discuss particular coding considerations pertaining to TRANS3.

2.2 Anisotropic Scattering Capability

The anisotropic scattering treatment described in Section 1.2, with the ray equations given by Eq. (10), has been programmed into TRANS3. The ray equations for isotropic, or transport-corrected isotropic, scattering given by Eq. (3) have also been programmed as an option in TRANS3. As discussed in Sections 1.1 and 1.2, the ray equations for isotropic scattering are decoupled, while those for anisotropic scattering are coupled; thus different computational schemes have been programmed in TRANS3 for the isotropic and anisotropic scattering cases.

Provision has been made within TRANS3 to generate the nine partial scattering cross sections $\bar{\Sigma}_s^i(g \rightarrow g)$, $i=1, \dots, 9$, defined in Section 1.2 for the 14 ray model, from group to group scattering Legendre coefficients which may be supplied in either the standard ANISIN or DTF-IV formats.

Storage requirements for the $9 \times G \times G$ matrix, where G is the number of energy groups, for each material is relatively negligible. The full anisotropic ray equations, given in matrix form by Eq. (10), however, represent a set of 14 coupled, linear equations. As one sweeps across the mesh, these equations could be solved iteratively, as originally suggested by Wagner(1). As will be discussed in Section 3.2, exploratory calculations with the code indicated that much faster convergence of the inner iterations, and substantial savings in run time, result from the direct solution of these 14 simultaneous equations as one sweeps through the mesh. In TRANS3 therefore, the inverted ray equation matrix A^{-1} is calculated and stored for each energy group in each material. This need be done only once at the beginning of any problem. Hence, $196 \times G$ locations are used for the storage of A^{-1} in each material. The working anisotropic ray equations as implemented in TRANS3 thus take the form

$$\tilde{\phi}^{g,n} = A^{-1} \tilde{S}^{g,n-1} \quad (26)$$

Use of the full anisotropic scattering model extends the run time by about a factor of four as compared to the use of the isotropic scattering model. Comparisons of exploratory calculations using the isotropic scattering option with calculations using the anisotropic model with isotropic cross section input data, showed the same number of inner iterations were required for convergence. The increase in run time for the anisotropic model can be attributed to the additional calculations required to accommodate the ray-to-ray scattering source terms.

2.3 Generalized Boundary Conditions

The generalized boundary conditions discussed in Section 1.3 have been programmed and implemented in the TRANS3 code. This capability allows the specification of boundary conditions at each point at which a ray penetrates the surface of the assembly for each energy group. The logic, which is implemented in subroutines TRAN3B and TRAN3C, represents a substantial portion of the coding of TRANS3.

The use of symmetry boundary conditions on the outer surfaces of appropriate layers of mesh blocks permits the use of the code in one- or two-dimensional geometries. This capability of running TRANS3 in one, two or three dimensions, within the same basic coding, is a particularly desirable one for design and analysis purposes.

2.4 Variable Mesh Capability

The variable mesh algorithm described in Section 1.4 has been programmed and implemented in the TRANS3 code for use with either isotropic or full anisotropic scattering. Exploratory calculations with a variable mesh used in all three dimensions of an assembly showed good results with mesh size variations by a factor of two.

It should be noted that the anisotropic ray matrix A which appears in Eq. (10) is dependent upon the shape and orientation of the mesh block as well as the partial anisotropic scattering cross sections. Because of the large reduction in run time, noted in Section 2.2, which results from the storage and use of the inverted ray equation matrix A^{-1} , it was decided to retain the practice in the case of variable mesh. In the current version of TRANS3, this requires the allocation of $196 \times G \times \text{NANSI}$ storage locations, where NANSI is the number of unique combinations of shape, orientation, and anisotropic scattering materials found in the spatial mesh blocks of the assembly. Thus, the combined use of the full anisotropic scattering model with the variable mesh capability can lead to large storage requirements. For extensive use of the combined capabilities, with resulting very large values of NANSI in a three-dimensional assembly, it might be appropriate to re-examine the programming logic philosophy.

The use of isotropic, or transport-corrected isotropic, scattering with the variable mesh capability creates as such storage problems. Indeed, the mesh block material parameters ($r_x^g, r_y^g, r_z^g, \Delta_x^g, \Delta_y^g, \Delta_z^g, \gamma_D^g, \delta_D^g$, etc.) do depend on the shape and orientation of the mesh block; but, since they are used in decoupled algebraic rather than matrix equations, the approach adopted has been to recalculate these parameters each time one sweeps through the mesh. As noted on the flow diagram in Appendix II, these material parameters are

normally stored only for the standard cubic mesh. In exploratory TRANS3 calculations with isotropic scattering and about 25% of mesh blocks of non-standard cubic shape, running time increased by approximately 30% over that for a uniform mesh.

2.5 Multigroup Capability

The DCR method with the fixed source/eigenvalue option, the extensions to full anisotropic scattering and variable mesh capability, and the use of generalized boundary conditions, has been implemented in TRANS3 within a variable multigroup formulation. As noted in Section 2.2, provision has been made in TRANS3 to generate the partial scattering cross sections from group-to-group scattering Legendre coefficients which may be supplied in either the standard ANISIN or DTF-IV formats. Energy group dependent block mesh sizes are not, however, permitted in TRANS3.

3.0 TASK 3 - EVALUATION OF NUMERICAL ALGORITHMS

Machine running time for any three-dimensional distribution code is sensitive to the specification of the numerical algorithms and logic utilized in the code. The following sections summarize the work done to date on selection of efficient computational algorithms in the TRANS3 code.

3.1 Spatial Mesh Sweeping Algorithms

Two spatial mesh sweeping algorithms, based on essentially different information updating schemes, have been evaluated in TRANS3. The first algorithm uses an information updating scheme wherein all the outgoing angular flux components for the mesh blocks are calculated and stored until a full spatial mesh sweep has been completed. All of the incoming angular flux components are then updated simultaneously. The second algorithm uses an instantaneous information updating scheme wherein as soon as the outgoing fluxes for a given mesh block are calculated, the incoming angular flux components for all adjacent mesh blocks are updated. Although not completely analogous, the two schemes may be likened to a Jacobi versus a Gauss-Seidel type iteration.

The second algorithm, based on instantaneous information updating leads to approximately a 25% faster convergence rate, and has been selected and implemented in TRANS3.

An added small improvement in convergence rate was realized by reversing the direction of the spatial sweep on alternate iterations. Currently, only two directions are being used and these appear adequate. Approximately a 10% faster convergence rate has been observed in exploratory calculations. This scheme, however, may potentially interfere with attempts at efficient dynamic data storage allocation schemes which are machine dependent.

3.2 Iterative Schemes

A major improvement in running time was achieved in the solution of the fully anisotropic ray equations by selection of an appropriate iterative scheme. It will be recalled from Section 1.2 that the anisotropic ray equations form a set of 14 fully coupled, linear equations. For example, the ray-to-ray scattering source for the outgoing angular flux component $\phi_{\ell}^{g,n}$ is given by Eq. (9), where, to preserve neutron balance within the region, one has

$$\begin{aligned}\bar{\psi}_{\ell}^{g,n-1} &= (1 + B_{\ell}^g) \psi_{\ell}^{g,n-1} - B_{\ell}^g \phi_{\ell \pm 3}^{g,n} \\ \bar{\psi}_m^{g,n-1} &= (1 + \beta_D^g) \psi_m^{g,n-1} - \beta_D^g \phi_{m \pm 4}^{g,n}\end{aligned}\tag{27}$$

where the parameters B_{ℓ}^g and β_D^g are defined by Eq. (A6) in Appendix I, and Eq. (9) follows from the analytic solution of the integral transport equation within the mesh block as given by Eq. (A14) in Appendix I.

A possible iterative scheme for the anisotropic ray equation (10) was originally suggested by Wagner(1), whereby instead of solving the system of equation explicitly for each inner iteration n , one accounts for the anisotropic scattering terms in an iterative way by using the anisotropic source term $S_{\ell}^{g,n-1}$, based on Eq. (27), from the previous inner iteration. An alternative scheme is to calculate and store the inverted ray equation matrix A^{-1} for each energy group in each material. This need be done only once at the beginning of any problem; and storage requirements, when standard cubic mesh blocks are employed, are minimal. The working ray equations then take the form of Eq. (26).

Both schemes were investigated in exploratory calculations in TRANS3. The two schemes require the same computation time and number of calculations per iteration. However, the difference in convergence rate was significant. In one sample three-dimensional calculation, at the end of 50 iterations the first scheme achieved convergence of the scalar flux to within only 0.08%; whereas at the end of only 4 iterations, the second scheme achieved convergence of the scalar flux to within 0.005%. This difference, which is representative of several exploratory calculations, represents more than an order of magnitude in running time. The second scheme, based on the calculation of the inverted ray matrix A^{-1} , has therefore been selected and implemented in TRANS3.

As indicated by Wagner in his original work(1), use of a group scaling factor as defined by Eq. (6) leads to substantial improvement in convergence rate of the iterative process. As noted in Section 1.4, rigorous use of an acceleration scheme when a variable mesh is employed would require the definition and application of an individual group scaling factor for each macroregion composed of mesh blocks of a given size and shape. In exploratory TRANS3 calculations, however, it has been found computationally convenient and efficient to use a single group scaling factor for the entire assembly to accelerate towards a nearly converged solution, and then set the group scaling factors to unity during the last few iterations to convergence.

4.0 TASK 4 - METHOD AND CODE VERIFICATION AND EVALUATION

This task was inactive during this report period.

5.0 TASK 5 - REPORT PREPARATION

This is the first in a series of technical progress reports on the development of a Three-Dimensional LMFBR Shielding Design and Analysis Code.

PROGRAM SCHEDULE

Task 1--Method Development, as specified in the proposed work, has been completed on schedule (milestone No. 1). Initial development of a special void streaming treatment, as described in Section 1.5, has been undertaken. Although not specified in the original work plan, plans are to pursue this development because of the relevance to program objectives. A preliminary working version of the code TRANS3 (Task 2--Code Development) has been completed (milestone No. 2) ahead of schedule. Work is proceeding on Task 3--Evaluation of Numerical Algorithms, according to schedule.

Approximate percentages of time and effort devoted by the investigators to the project are indicated below, as well as a forecast of future effort.

	<u>6/1/74 TO DATE</u>		<u>REMAINING PERIOD</u>		<u>TOTAL</u>	
	<u>Man Months</u>	<u>Percent</u>	<u>Man Months</u>	<u>Percent</u>	<u>Man Months</u>	<u>Percent</u>
Principal Investigator (C.G.Poncelet)	1	20%	4	80%	5	100%
Graduate Student (J.A.Bucholz)	4	33%	8	67%	12	100%

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APPENDIX I

TRANS3 WORKING EQUATIONS

The purpose of this appendix is to show in detail the iterative equations used in the TRANS3 code. For the sake of presentation, these equations may be grouped into eight sets:

- (1) Basic parameter definitions;
- (2) Definition of the partial scattering cross sections peculiar to the TRANS3 code;
- (3) Generalized boundary conditions;
- (4) Equations for the scalar flux;
- (5) Equations for the isotropic and anisotropic ray-source terms;
- (6) The isotropic and anisotropic ray equations;
- (7) Equations defining the group scaling factor; and
- (8) A definition of the eigenvalue as given by the power method.

Throughout this Appendix superscripts n and g shall denote the inner iteration index, and energy group number, respectively.

Equation numbers shown on the TRANS3 flow diagram in Appendix II refer to equations in this Appendix.

1. Basic Parameter Definitions

The following definitions have been used within the code and throughout this Appendix for brevity. In the case of Eq. (A6), the limit function is chosen at the point indicated so as to avoid machine round-off error. The subscripts l and m refer to the corresponding direction or ray where, for example, $l=1,2,3$ refers to directions x,y,z and/or the corresponding normally directed angular flux components.

$$\Gamma_l^g = e^{-\sum_T^g h_l} \quad (A-1)$$

$$\gamma_D^g = e^{-\sum_T^g h_{DP}} \quad (A-2)$$

$$\text{where } h_{DP} = \min\{h_1\sqrt{3}, h_2\sqrt{3}, h_3\sqrt{3}\} \quad (A-3)$$

$$\Delta_l^g = \begin{cases} \frac{1 - \Gamma_l^g}{\sum_T^g} & \text{if } \sum_T^g h_l > 2 \times 10^{-7} \\ h_l & \text{if } \sum_T^g h_l \leq 2 \times 10^{-7} \end{cases} \quad (A-4)$$

$$\delta_D^g = \begin{cases} \frac{1 - \gamma_D^g}{\sum_T^g} & \text{if } \sum_T^g h_{DP} > 2 \times 10^{-7} \\ h_{DP} & \text{if } \sum_T^g h_{DP} \leq 2 \times 10^{-7} \end{cases} \quad (A-5)$$

$$B_{\ell}^g = \begin{cases} \left[\left(\frac{1}{\sum_{\tau}^g h_{\ell}} \right) - \left(\frac{1}{1 - \Gamma_{\ell}^g} \right) \right] & \text{if } \sum_{\tau}^g h_{\ell} \geq 0.001 \\ - \left(\frac{1 + \sum_{\tau}^g h_{\ell}}{2 + \sum_{\tau}^g h_{\ell}} \right) & \text{if } \sum_{\tau}^g h_{\ell} < 0.001 \end{cases}$$

(A-6)

$$\beta_{\text{D}}^g = \begin{cases} \left[\left(\frac{1}{\sum_{\tau}^g h_{\text{DP}}} \right) - \left(\frac{1}{1 - \gamma_{\text{D}}^g} \right) \right] & \text{if } \sum_{\tau}^g h_{\text{DP}} \geq 0.001 \\ - \left(\frac{1 + \sum_{\tau}^g h_{\text{DP}}}{2 + \sum_{\tau}^g h_{\text{DP}}} \right) & \text{if } \sum_{\tau}^g h_{\text{DP}} < 0.001 \end{cases}$$

$$a_p^g = - \left(\beta_{\text{D}}^g \delta_{\text{D}}^g + 2[B_1^g \Delta_1^g + B_2^g \Delta_2^g + B_3^g \Delta_3^g] \right) \quad (\text{A-7})$$

Several other parameters (α , λ , $\theta^{g,n}$) are used to differentiate between fixed source and eigenvalue calculations. For a fixed source calculation $\alpha=1$; λ is a known value (must be specified by the user, otherwise defaulted to unity); and $\theta^{g,n} = \phi^{g,n}$, the local scalar flux. For an eigenvalue calculation $\alpha=0$; $\lambda=1.0$; and $\theta^{g,n}$ denotes the local scalar flux from the previous outer iteration. In this case, λ denotes the calculated eigenvalue.

2. Definitions of the Partial Scattering Cross Sections Peculiar to the TRANS3 Code

The partial scattering cross sections employed in the 14 ray method are:

$$\Sigma_s^1(g' \rightarrow g) = 2\pi \int_{6/7}^1 \Sigma_s^{g' \rightarrow g}(\mu) d\mu$$

$$\Sigma_s^3(g' \rightarrow g) = \frac{2\pi}{4} \int_{2/7}^{6/7} \Sigma_s^{g' \rightarrow g}(\mu) d\mu$$

$$\Sigma_s^5(g' \rightarrow g) = \frac{2\pi}{4} \int_{-2/7}^{2/7} \Sigma_s^{g' \rightarrow g}(\mu) d\mu$$

$$\Sigma_s^7(g' \rightarrow g) = \frac{2\pi}{4} \int_{-6/7}^{-2/7} \Sigma_s^{g' \rightarrow g}(\mu) d\mu$$

$$\Sigma_s^9(g' \rightarrow g) = 2\pi \int_{-1}^{-6/7} \Sigma_s^{g' \rightarrow g}(\mu) d\mu$$

$$\Sigma_s^2(g' \rightarrow g) = \frac{2\pi}{3} \int_{3/7}^{6/7} \Sigma_s^{g' \rightarrow g}(\mu) d\mu$$

$$\Sigma_s^4(g' \rightarrow g) = \frac{2\pi}{3} \int_0^{3/7} \Sigma_s^{g' \rightarrow g}(\mu) d\mu$$

$$\Sigma_s^6(g' \rightarrow g) = \frac{2\pi}{3} \int_{-3/7}^0 \Sigma_s^{g' \rightarrow g}(\mu) d\mu \quad (\text{A-8})$$

$$\Sigma_s^8(g' \rightarrow g) = \frac{2\pi}{3} \int_{-6/7}^{-3/7} \Sigma_s^{g' \rightarrow g}(\mu) d\mu$$

$$\Sigma_s^{g' \rightarrow g} = 2\pi \int_{-1}^1 \Sigma_s^{g' \rightarrow g}(\mu) d\mu$$

where

In Eq. (A8), μ is cosine of the scattering angle and $\Sigma_s^{g' \rightarrow g}(\mu)$ are the group-to-group differential scattering cross sections. If the ray-to-ray scattering probabilities are not defined in an integral sense, the fully developed 14 ray method may be collapsed to the P-1 model originally proposed by Wagner(1) by using:

$$\Sigma_s^1(g' \rightarrow g) = \frac{1}{14} \left[\Sigma_s^{g' \rightarrow g} + \Sigma_{s, P_1}^{g' \rightarrow g} \right]$$

$$\Sigma_s^3(g' \rightarrow g) = \frac{1}{14} \left[\Sigma_s^{g' \rightarrow g} + \frac{1}{\sqrt{3}} \Sigma_{s, P_1}^{g' \rightarrow g} \right]$$

$$\Sigma_s^5(g' \rightarrow g) = \frac{1}{14} \left[\Sigma_s^{g' \rightarrow g} \right]$$

$$\Sigma_s^7(g' \rightarrow g) = \frac{1}{14} \left[\Sigma_s^{g' \rightarrow g} - \frac{1}{\sqrt{3}} \Sigma_{s, P_1}^{g' \rightarrow g} \right]$$

$$\Sigma_s^9(g' \rightarrow g) = \frac{1}{14} \left[\Sigma_s^{g' \rightarrow g} - \Sigma_{s, P_1}^{g' \rightarrow g} \right]$$

$$\Sigma_s^2(g' \rightarrow g) = \frac{1}{14} \left[\Sigma_s^{g' \rightarrow g} + \frac{1}{\sqrt{3}} \Sigma_{s, P_1}^{g' \rightarrow g} \right]$$

$$\Sigma_s^4(g' \rightarrow g) = \frac{1}{14} \left[\Sigma_s^{g' \rightarrow g} + \frac{1}{3} \Sigma_{s, P_1}^{g' \rightarrow g} \right]$$

$$\Sigma_s^6(g' \rightarrow g) = \frac{1}{14} \left[\Sigma_s^{g' \rightarrow g} - \frac{1}{3} \Sigma_{s, P_1}^{g' \rightarrow g} \right]$$

$$\Sigma_s^8(g' \rightarrow g) = \frac{1}{14} \left[\Sigma_s^{g' \rightarrow g} - \frac{1}{\sqrt{3}} \Sigma_{s, P_1}^{g' \rightarrow g} \right]$$

(A-9)

For fissioning media, one additional parameter may be defined:

$$\bar{\Sigma}_s^i(g' \rightarrow g) = \Sigma_s^i(g' \rightarrow g) + \left(\frac{\alpha}{14} \right) \left(\frac{1}{\lambda} \right) \kappa^2 \nu^{g'} \Sigma_F^{g'}$$

(A-10)

3. Generalized Boundary Conditions

For illustrative purposes, consider an element (j,k) on the $i=I$ surface of an assembly measuring $I \times J \times K$. In the event that $j \neq 1$, $j \neq J$, $k \neq 1$ and $k \neq K$, the generalized boundary condition for Ψ_1 , ψ_1 , ψ_3 , ψ_6 , and ψ_8 may be summarized in tabular form as:

	VACUUM	REFLECTION WITH ALBEDO	PERIODIC	SPECIFIED SOURCE
$\Psi_1^g(I, j, k)$	0	$\Phi_1^g(I, j, k) \beta_{p_{1,I}}^g(j, k)$	$\Phi_4^g(1, j, k)$	$*\Psi_1^g(I, j, k)$
$\psi_1^g(I, j, k)$	0	$\phi_1^g(I, j, k) \beta_{p_{1,I}}^g(j, k)$	$\psi_5^g(1, j+1, k+1)$	$*\psi_1^g(I, j, k)$
$\psi_3^g(I, j, k)$	0	$\phi_3^g(I, j, k) \beta_{p_{3,I}}^g(j, k)$	$\psi_7^g(1, j-1, k+1)$	$*\psi_3^g(I, j, k)$
$\psi_6^g(I, j, k)$	0	$\phi_6^g(I, j, k) \beta_{p_{6,I}}^g(j, k)$	$\psi_2^g(1, j-1, k-1)$	$*\psi_6^g(I, j, k)$
$\psi_8^g(I, j, k)$	0	$\phi_8^g(I, j, k) \beta_{p_{8,I}}^g(j, k)$	$\psi_4^g(1, j+1, k-1)$	$*\psi_8^g(I, j, k)$

(A-11)

where $\beta_{p_{3,I}}^g(j, k)$ is the albedo for group g at point p_3 of the element (j, k) on the $i=I$ surface of the assembly and where $*\psi_3^g(I, j, k)$ is the specified source for the given ray.

In the interior of the assembly, the continuity of rays from one block to the next gives rise to the following conditions:

$$\begin{array}{ll}
 \text{IF } (i \neq I) \quad \Psi_1^{g,n-1} = \Phi_4^{g,n-1}(i+1, j, k) & \text{IF } ((i \neq I) \& (j \neq J) \& (k \neq K)) \quad \psi_1^{g,n-1} = \phi_5^{g,n-1}(i+1, j+1, k+1) \\
 \text{IF } (j \neq J) \quad \Psi_2^{g,n-1} = \Phi_5^{g,n-1}(i, j+1, k) & \text{IF } ((i \neq I) \& (j \neq J) \& (k \neq K)) \quad \psi_2^{g,n-1} = \phi_6^{g,n-1}(i-1, j+1, k+1) \\
 \text{IF } (k \neq K) \quad \Psi_3^{g,n-1} = \Phi_6^{g,n-1}(i, j, k+1) & \text{IF } ((i \neq I) \& (j \neq J) \& (k \neq K)) \quad \psi_3^{g,n-1} = \phi_7^{g,n-1}(i+1, j-1, k+1) \\
 \text{IF } (i \neq I) \quad \Psi_4^{g,n-1} = \Phi_1^{g,n-1}(i-1, j, k) & \text{IF } ((i \neq I) \& (j \neq J) \& (k \neq K)) \quad \psi_4^{g,n-1} = \phi_8^{g,n-1}(i-1, j-1, k+1) \\
 \text{IF } (j \neq J) \quad \Psi_5^{g,n-1} = \Phi_2^{g,n-1}(i, j-1, k) & \text{IF } ((i \neq I) \& (j \neq J) \& (k \neq K)) \quad \psi_5^{g,n-1} = \phi_1^{g,n-1}(i-1, j-1, k-1) \\
 \text{IF } (k \neq K) \quad \Psi_6^{g,n-1} = \Phi_3^{g,n-1}(i, j, k-1) & \text{IF } ((i \neq I) \& (j \neq J) \& (k \neq K)) \quad \psi_6^{g,n-1} = \phi_2^{g,n-1}(i+1, j-1, k-1) \\
 & \text{IF } ((i \neq I) \& (j \neq J) \& (k \neq K)) \quad \psi_7^{g,n-1} = \phi_3^{g,n-1}(i-1, j+1, k-1) \\
 & \text{IF } ((i \neq I) \& (j \neq J) \& (k \neq K)) \quad \psi_8^{g,n-1} = \phi_4^{g,n-1}(i+1, j+1, k-1)
 \end{array} \tag{A-12}$$

where $\psi_{\ell}^{g,n-1}$ and $\psi_m^{g,n-1}$ denote $\psi_{\ell}^{g,n-1}(i, j, k)$ and $\psi_m^{g,n-1}(i, j, k)$.

4. Equations for the Scalar Flux

Within any given block the scalar flux is defined by:

$$\phi^{g,n} = \left(\frac{1}{14}\right) \left[\sum_{\ell=1}^6 (\overline{\Psi}_{\ell}^{g,n-1}) + \sum_{m=1}^8 (\overline{\psi}_m^{g,n-1}) \right] \quad (A-13)$$

where

$$\begin{aligned} \overline{\Psi}_{\ell}^{g,n} &= \overline{\Phi}_{\ell+3}^{g,n} = \Psi_{\ell}^{g,n} + B_{\ell}^g (\Psi_{\ell}^{g,n} - \Phi_{\ell+3}^{g,n}) & \ell = 1, 2, 3 \\ \overline{\Psi}_{\ell}^{g,n} &= \overline{\Phi}_{\ell-3}^{g,n} = \Psi_{\ell}^{g,n} + B_{\ell}^g (\Psi_{\ell}^{g,n} - \Phi_{\ell-3}^{g,n}) & \ell = 4, 5, 6 \\ \overline{\psi}_m^{g,n} &= \overline{\Phi}_{m+4}^{g,n} = \psi_m^{g,n} + \beta_0^g (\psi_m^{g,n} - \Phi_{m+4}^{g,n}) & m = 1, 2, 3, 4 \\ \overline{\psi}_m^{g,n} &= \overline{\Phi}_{m-4}^{g,n} = \psi_m^{g,n} + \beta_0^g (\psi_m^{g,n} - \Phi_{m-4}^{g,n}) & m = 5, 6, 7, 8 \end{aligned} \quad (A-14)$$

In the case of isotropic scattering, the scalar flux may be written in closed form as:

$$\begin{aligned} \phi^{g,n} &= \left\{ a_p^g \left[Q_{ext} - \left(\sum_s^{g \rightarrow g} + \left(\frac{\alpha}{\lambda} \right) \kappa^g \nu^g \sum_F^g \right) \phi^{g,n-1} + \right. \right. \\ &\quad \left. \left. + \sum_{g'=1}^6 \left\{ \sum_s^{g' \rightarrow g} \phi^{g',n-1} + \left(\frac{1}{\lambda} \right) \kappa^g \nu^g \sum_F^{g'} \phi^{g',n-1} \right\} \right] + \left[\left(\sum_{\ell=1}^6 \frac{\Delta_{\ell}^g}{h_{\ell}} \Psi_{\ell}^{g,n-1} \right) + \right. \right. \\ &\quad \left. \left. + \frac{\delta_0^g}{h_{0p}} \left(\sum_{m=1}^8 \psi_m^{g,n-1} \right) \right] \right\} \left[\frac{1}{14 - a_p^g \left(\sum_s^{g \rightarrow g} + \left(\frac{\alpha}{\lambda} \right) \kappa^g \nu^g \sum_F^g \right)} \right] \end{aligned} \quad (A-15)$$

5. Equations for the Isotropic and Anisotropic Ray-Source Terms

In the full anisotropic scattering model, each outgoing angular flux component will have its own ray-to-ray scattering sources in addition to whatever isotropic sources may be present. The iterative ray equations within a mesh block may then be written in the matrix form of Eq. (10) in the main text where, for example, the source component $S_1^{g,n-1}$ associated with $\phi_1^{g,n}$ is given by:

$$\begin{aligned}
 S_1^{g,n-1} = & \Gamma_1^g \Psi_4^{g,n-1} + \Delta_1^g \left[F^{g,n-1} + \sum_{g' \neq 1}^6 \left\{ \bar{\Sigma}_s^{g'}(g \rightarrow g') \bar{\Psi}_4^{g',n-1} + \right. \right. \\
 & + \bar{\Sigma}_s^{g'}(g' \rightarrow g) [\bar{\Psi}_2^{g',n-1} + \bar{\Psi}_4^{g',n-1} + \bar{\Psi}_5^{g',n-1} + \bar{\Psi}_7^{g',n-1}] + \bar{\Sigma}_s^{g'}(g' \rightarrow g) [\bar{\Psi}_2^{g',n-1} + \bar{\Psi}_3^{g',n-1} + \bar{\Psi}_5^{g',n-1} + \bar{\Psi}_6^{g',n-1}] + \\
 & + \bar{\Sigma}_s^{g'}(g' \rightarrow g) [\bar{\Psi}_1^{g',n-1} + \bar{\Psi}_3^{g',n-1} + \bar{\Psi}_6^{g',n-1} + \bar{\Psi}_8^{g',n-1}] + \bar{\Sigma}_s^{g'}(g' \rightarrow g) \bar{\Psi}_i^{g',n-1} \left. \right\} + \left\{ B_1^{g'} \bar{\Sigma}_s^{g'}(g \rightarrow g') \phi_1^{g',n-1} + \right. \\
 & + B_0^{g'} \bar{\Sigma}_s^{g'}(g \rightarrow g) [\phi_1^{g',n-1} + \phi_3^{g',n-1} + \phi_6^{g',n-1} + \phi_8^{g',n-1}] + B_2^{g'} \bar{\Sigma}_s^{g'}(g \rightarrow g) [\phi_2^{g',n-1} + \phi_5^{g',n-1}] + \\
 & \left. \left. + B_3^{g'} \bar{\Sigma}_s^{g'}(g \rightarrow g) [\phi_3^{g',n-1} + \phi_6^{g',n-1}] + B_0^{g'} \bar{\Sigma}_s^{g'}(g \rightarrow g) [\phi_2^{g',n-1} + \phi_4^{g',n-1} + \phi_5^{g',n-1} + \phi_7^{g',n-1}] + B_1^{g'} \bar{\Sigma}_s^{g'}(g \rightarrow g) \phi_4^{g',n-1} \right\} \right]
 \end{aligned} \tag{A-16}$$

where the isotropic source term $F^{g,n}$ is given by

$$\begin{aligned}
 F^{g,n} = & Q_{\text{ext}}^g + \sum_{g' \neq 1}^6 \left\{ \frac{1}{\lambda} \kappa^g \nu^{g'} \bar{\Sigma}_F^{g'} \theta^{g',n} + \bar{\Sigma}_s^{g' \rightarrow g} \phi^{g',n} \right\} \quad \text{for isotropic media} \\
 F^{g,n} = & Q_{\text{ext}}^g + (1-\alpha) \sum_{g' \neq 1}^6 \left\{ \frac{1}{\lambda} \kappa^g \nu^{g'} \bar{\Sigma}_F^{g'} \theta^{g',n} \right\} \quad \text{for anisotropic media}
 \end{aligned} \tag{A-17}$$

Equations for source components associated with other rays can be developed in a similar way. They are not reproduced here for the sake of compactness.

6. The Isotropic and Anisotropic Ray Equations

In the case of the full anisotropic scattering model, the iterative ray equations may be written in the form of Eq. (10) in the main text where A is the ray equation matrix for the given mesh block and energy group. It measures 14×14 and is dependent on the partial scattering cross sections and the size and shape of the block. Since it is the inverted ray equation matrix (A^{-1}) which is stored, the working equations are simply:

$$\phi^{g,n} = (A^{-1}) S^{g,n-1} \quad (A-18)$$

The form of the matrices A and A^{-1} are not reproduced here explicitly for the sake of brevity. The elements of the matrix A can be generated readily by reference to the procedure outlined in the main text, and to the ray source terms above. In the case of isotropic scattering, the iterative ray equations for the outgoing angular flux components may be written simply as:

$$\begin{aligned} \phi_l^{g,n} &= \Gamma_l^g \psi_{l+3}^{g,n-1} + \Delta_l^g F^{g,n} & l = 1, 2, 3 \\ \phi_l^{g,n} &= \Gamma_l^g \psi_{l-3}^{g,n-1} + \Delta_l^g F^{g,n} & l = 4, 5, 6 \end{aligned} \quad (A-19)$$

$$\phi_m^{g,n} = \gamma_0^g \psi_{m+4}^{g,n-1} + \delta_0^g F^{g,n} \quad m = 1, 2, 3, 4$$

$$\phi_m^{g,n} = \gamma_0^g \psi_{m-4}^{g,n-1} + \delta_0^g F^{g,n} \quad m = 5, 6, 7, 8 \quad (A-20)$$

7. Equations Defining the Group Scaling Factor

The group scaling factor $f^{g,n}$ is an acceleration parameter which is calculated and applied at the end of the n^{th} inner iteration so as to insure neutron balance for each energy group throughout the entire assembly or macroregion, and is defined by Eq. (6) of the main text. The total leakage, group removal and source terms are given by:

$$\begin{aligned} \mathcal{L}_{\Sigma c}^g = & \left(\frac{1}{4} \right) \left\{ \sum_i \sum_j \sum_k \sum_l \frac{V_{ol}(i,j,k)}{h_x(i,j,k)} \left[\Phi_l^{g,n}(i,j,k) - \Psi_l^{g,n-1}(i,j,k) \right] + \right. \\ & \left. + \sum_i \sum_j \sum_k \sum_m \frac{V_{ol}(i,j,k)}{h_{op}(i,j,k)} \left[\Phi_m^{g,n}(i,j,k) - \Psi_m^{g,n-1}(i,j,k) \right] \right\} \quad (\text{A-21}) \end{aligned}$$

Note that the summations are taken over only those normal and diagonal rays which penetrate the outside surface of the assembly or macroregion.

$$\begin{aligned} \mathcal{L}_E^g(i,j,k) = & \left(\sum_r \mathcal{L}_r^g(i,j,k) - \sum_s \mathcal{L}_s^{g+g}(i,j,k) - \left(\frac{\alpha}{\lambda} \right) \mathcal{L}^g \mathcal{V}^g \sum_F \mathcal{L}_F^g(i,j,k) \right) \Phi^{g,n}(i,j,k) \\ \mathcal{L}_\tau^g(i,j,k) = & Q_{ext}^g(i,j,k) - \left(\sum_s \mathcal{L}_s^{g+g}(i,j,k) + \left(\frac{\alpha}{\lambda} \right) \mathcal{L}^g \mathcal{V}^g \sum_F \mathcal{L}_F^g(i,j,k) \right) \Phi^{g,n}(i,j,k) + \\ & + \sum_{g'=1}^6 \left\{ \sum_s \mathcal{L}_s^{g'+g}(i,j,k) \Phi^{g',n}(i,j,k) + \left(\frac{1}{\lambda} \right) \mathcal{L}^g \mathcal{V}^{g'} \sum_F \mathcal{L}_F^{g'}(i,j,k) \Phi^{g',n}(i,j,k) \right\} \quad (\text{A-22}) \end{aligned}$$

From these terms the group scaling factor $f^{g,n}$ may be computed as:

$$f^{g,n} = \left[\sum_i \sum_j \sum_k V_{ol}(i,j,k) \mathcal{L}_\tau^g(i,j,k) \right] / \left[\sum_i \sum_j \sum_k V_{ol}(i,j,k) \mathcal{L}_E^g(i,j,k) + \mathcal{L}_{\Sigma c}^g \right] \quad (\text{A-23})$$

Note that these summations extend over all blocks (i,j,k) within the assembly or macroregion.

8. Definition of the Eigenvalue as Given by the Power Method

Using the power method and letting $\phi^{g,N}$ denote the scalar flux of the N^{th} outer iteration, the eigenvalue λ_N is given by

$$\lambda_N = \frac{\sum_{i=1}^I \sum_{j=1}^J \sum_{k=1}^K \sum_{g=1}^G Vol(i,j,k) \nu^g \sum_F^g(i,j,k) \phi^{g,N}(i,j,k)}{\sum_{i=1}^I \sum_{j=1}^J \sum_{k=1}^K \sum_{g=1}^G Vol(i,j,k) \nu^g \sum_F^g(i,j,k) \overline{\phi^{g,N-1}}(i,j,k)} \quad (\text{A-24})$$

where $\overline{\phi^{g,N-1}}(i,j,k)$ has been normalized such that

$$\overline{\phi^{g,N-1}}(i,j,k) = \phi^{g,N-1}(i,j,k) / \left[\sum_{i=1}^I \sum_{j=1}^J \sum_{k=1}^K \sum_{g=1}^G \phi^{g,N-1}(i,j,k) \right] \quad (\text{A-25})$$

and where $\phi^{g,N}(i,j,k)$ has not yet been normalized.

APPENDIX II

TRANS3 FLOW DIAGRAM