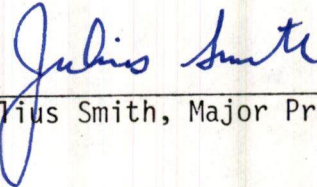


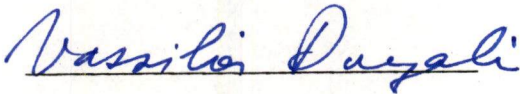
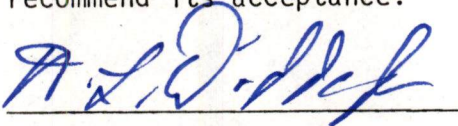
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I am submitting herewith a thesis written by John E. Aull entitled "Acceleration of the Inner Iteration of the DOT-IV Transport Code Using a New Source Correction Scheme." I recommend that it be accepted in partial fulfillment of the requirements for the degree of Master of Science, with a major in Mathematics.

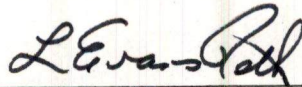


Julius Smith, Major Professor

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ACCELERATION OF THE INNER ITERATION OF THE
DOT-IV TRANSPORT CODE USING A NEW
SOURCE CORRECTION SCHEME

A Thesis
Presented for the
Master of Science
Degree
The University of Tennessee, Knoxville

John E. Aull
December 1979

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ABSTRACT

A detailed description of the steady state Boltzmann transport equation is given. Then the discrete ordinates method of solving the transport equation is described.

The conventional rebalance method, the source correction scheme of rebalance and a new source correction scheme involving a correction equation with a modified flow term are derived. Difference equations for each version of the source correction scheme are presented. The different versions of the source correction scheme and the conventional rebalance method are compared on several test problems in one- and two-dimensional slab geometry.

Results are shown which demonstrate that the new source correction scheme is superior to the conventional rebalance method. It is also seen that the new source correction scheme is compatible when used with a weighted difference formulation in the inner iteration of the transport solution.

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INTRODUCTION

The Boltzmann transport equation is universally recognized as an accurate mathematical model for describing the transport of neutral particles (i.e., neutrons and gammas) in nuclear reactor systems. The complexity of the Boltzmann equation (to be described in the next section) and the systems for which it is used necessitate the use of numerical approximation methods to obtain a solution. One such method is the discrete ordinates approach.¹

Several computer codes have been developed which use the discrete ordinates method for solving neutron and gamma transport problems.² These codes employ iterative solution techniques which can be quite expensive even on the latest generation of large, fast digital computers. Much work has been done to find ways to accelerate the convergence of the iterative techniques in order to reduce computing costs.

The objective of this thesis is to investigate a particular acceleration procedure, called the source correction scheme (SCS), which was developed at Los Alamos Scientific Laboratory by Alcouffe and his associates.³ Specifically, a somewhat novel variation of the SCS was implemented in the DOT-IV code.⁴ It was then evaluated by comparing numerical results obtained by the new approach with results obtained by conventional acceleration procedures.

In the next section a detailed description of the Boltzmann transport equation is given. Then a description of how the transport equation is solved using the discrete ordinates method is presented.

Section IV contains a description of how the source correction scheme is used to accelerate convergence. A statement of the problem solved in this thesis is given in Sect. III. Sections V and VI contain, respectively, numerical results and conclusions about the success of the method.

I. THE BOLTZMANN TRANSPORT EQUATION

A. The Boltzmann Transport Equation

The steady state Boltzmann transport equation is

$$\begin{aligned} & \bar{\Omega} \cdot \nabla \psi(\bar{r}, \bar{\Omega}, E) + \sigma(\bar{r}, E) \psi(\bar{r}, \bar{\Omega}, E) \\ &= \iint \sigma_s(\bar{r}, \bar{\Omega}' \rightarrow \bar{\Omega}, E' \rightarrow E) \psi(\bar{r}, \bar{\Omega}', E') dE' d\bar{\Omega}' \\ &+ \chi(E) \iint v \sigma_f(\bar{r}, E') \psi(\bar{r}, \bar{\Omega}', E') dE' d\bar{\Omega}' \\ &+ Q(\bar{r}, \bar{\Omega}, E) .^1 \end{aligned} \tag{1}$$

In this equation ψ is the directional flux which is expressed in units of number of neutrons per unit volume per unit energy per unit solid angle. ψ is a function of a position vector $\bar{r}$, a unit direction vector in velocity space, $\bar{\Omega}$, and energy E . The unit direction vector $\bar{\Omega} = (\tau, \theta)$ is an ordered pair of angles as shown in Fig. 1. In Eq. (1) the terms on the left side represent losses of neutrons and the terms on the right side represent sources of neutrons.

The first term represents losses due to leakage. In the second term, $\sigma(\bar{r}, E)$ is the total macroscopic cross section. It represents the probability that a neutron be removed through interaction with a nucleus. So the second term in Eq. (1) represents loss due to scattering and absorption.

The first term on the right represents the source of neutrons due to scattering. The symbol, $\sigma_s(\bar{r}, \bar{\Omega}' \rightarrow \bar{\Omega}, E' \rightarrow E)$, represents the differential scattering cross section. The direction of a neutron before scattering

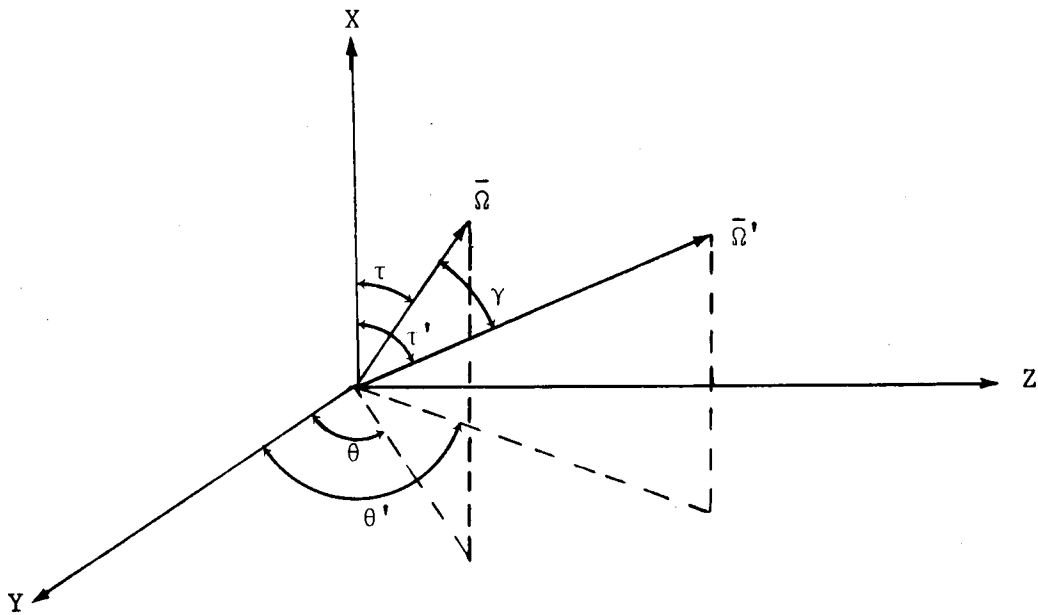


Fig. 1. The Unit Vectors $\bar{\Omega}$ and $\bar{\Omega}'$.

occurs is $\bar{\Omega}'$. The direction after scattering has occurred is $\bar{\Omega}$. E' and E represent the energy of a neutron before and after scattering.

$\sigma_s(\bar{r}, \bar{\Omega}' \rightarrow \bar{\Omega}, E' \rightarrow E)$ represents the probability of a neutron scattering from the direction $\bar{\Omega}'$ with energy E' to the direction $\bar{\Omega}$ with energy E . So the first term on the right side of Eq. (1) represents the source due to scattering from all directions and energies to the direction $\bar{\Omega}$ and energy E .

The second term on the right side of Eq. (1) represents the fission source. $\chi(E)$ is the fission spectrum. It is the probability that a neutron emitted as a result of fission will be at the energy E . The symbol ν represents the number of neutrons emitted per fission.

$\sigma_f(\bar{r}, E')$ represents the probability that fission will take place at the position $\bar{r}$ for an incoming neutron of energy E' . So the second term on

the right side of Eq. (1) represents the source of neutrons due to fission.

The last term of Eq. (1) represents an extraneous nonfissile source. There are two large classes of problems that are solved using Eq. (1). They are eigenvalue problems and fixed source problems.

One type of fixed source problem deals with the calculation of the flux in a reactor shield. Shields usually do not contain fissile material so a shielding problem is usually characterized by the absence of the fission term in Eq. (1). The extraneous source, Q , is always present in a shielding problem.

An eigenvalue problem is characterized by the absence of the extraneous source Q . The scattering source term can then be transferred to the left side of Eq. (1) and it can be written in linear operator form as

$$L\psi(\bar{r}, \bar{\Omega}, E) = \frac{1}{k} M\psi(\bar{r}, \bar{\Omega}, E) \quad (2)$$

where

$$L\psi(\bar{r}, \bar{\Omega}, E) = [\bar{\Omega} \cdot \nabla + \sigma(\bar{r}, E)] \psi(\bar{r}, \bar{\Omega}, E) - \iint \sigma_s(\bar{r}, \bar{\Omega}' \rightarrow \bar{\Omega}, E' \rightarrow E) \psi(\bar{r}, \bar{\Omega}', E') d\bar{\Omega}' dE' \quad (3)$$

and

$$M\psi(\bar{r}, \bar{\Omega}, E) = \chi(E) \iint v\sigma_f(\bar{r}, E') \psi(\bar{r}, \bar{\Omega}', E') dE' d\bar{\Omega}'$$

and k is an eigenvalue.

B. The Transport Equation in Slab Geometry

In this work two special cases of the Boltzmann transport equation are considered. The two special cases are the transport equation in one-dimensional slab geometry and the transport equation in two-dimensional slab geometry.

In one-dimensional slab geometry the flux ψ is a function of one space variable, x , and one angular variable. The only angle in Fig. 1, page 4, that can be used to denote direction with respect to the X axis is the angle τ . Instead of the angle τ the cosine, $\mu = \cos \tau$, is used. Thus, the steady state Boltzmann transport equation in one-dimensional slab geometry is

$$\begin{aligned}
 & \mu \frac{\partial}{\partial x} \psi(x, \mu, E) + \sigma(x, E) \psi(x, \mu, E) \\
 &= \chi(E) \int_0^{\infty} \int_{-1}^1 \left(\frac{1}{2} \right) v \sigma_f(x, E') \psi(x, \mu', E') d\mu' dE' \\
 &+ \frac{1}{4\pi} \int_0^{\infty} \int_0^{2\pi} \int_{-1}^1 \sigma_s(x, \mu_0, E' \rightarrow E) \psi(x, \mu', E') d\mu' d\theta' dE' \\
 &+ Q(x, \mu, E)
 \end{aligned} \tag{4}$$

where

$$\mu_0 = \cos \gamma \tag{5}$$

and γ is the angle between the direction before scattering and the direction after scattering.¹ The angle γ is shown in Fig. 1, page 4.

For the case of two dimensional slab geometry the flux is a function of the position variables x and y . It is also a function of two angles. The two angles are τ and θ as seen in Fig. 1. As in the one dimensional case the variable $\mu = \cos \tau$ is used. However the angular variable, θ , is used because it varies from 0 to 2π . The transport equation in two-dimensional slab geometry is

$$\begin{aligned}
 & \sqrt{1 - \mu^2} \cos \theta \frac{\partial \psi}{\partial y}(x, y, \mu, \theta, E) + \mu \frac{\partial \psi}{\partial x}(x, y, \mu, \theta, E) \\
 & + \sigma(x, y, E) \psi(x, y, \mu, \theta, E) \\
 & = \chi(E) \int_0^\infty \int_0^{2\pi} \int_{-1}^1 \left(\frac{1}{4\pi} \right) v \sigma_f(x, y, E') \psi(x, y, \mu', \theta', E') d\mu' d\theta' dE' \\
 & + \int_0^\infty \int_0^{2\pi} \int_{-1}^1 \left(\frac{1}{4\pi} \right) \sigma_s(x, y, \mu_0, E' \rightarrow E) \psi(x, y, \mu', \theta', E') d\mu' d\theta' dE' \\
 & + Q(x, y, \mu, \theta, E)
 \end{aligned}$$

where μ_0 is the same as in Eq. (5).⁵

II. SOLVING THE BOLTZMANN TRANSPORT EQUATION

A. Inner and Outer Iterations

The solution of Eq. (1) involves the use of two nested iterations called outer and inner iterations which will be described shortly. The first step in solving the transport equation is to discretize the energy variable E . Energy theoretically varies from zero to infinity in the transport equation but a maximum energy of 10 MeV is usually used in practice.² So the energy variable is discretized into G energy groups each of width ΔE_g . E_0 is the highest possible energy. E_G is the lowest energy. Thus the g th energy group, $\Delta E_g = E_{g-1} - E_g$. With this discretization Eq. (1) can be written as a set of G equations,

$$\begin{aligned} \bar{\Omega} \cdot \nabla \psi_g(\bar{r}, \bar{\Omega}) + \sigma_g(\bar{r}) \psi_g(\bar{r}, \bar{\Omega}) = & \int \sum_{g'=1}^G \sigma_{sg \rightarrow g}(\bar{r}, \bar{\Omega}' \rightarrow \bar{\Omega}) \psi_{g'}(\bar{r}, \bar{\Omega}') d\bar{\Omega}' \\ & + \chi_g \int \sum_{g'=1}^G \nu \sigma_{fg'}(\bar{r}) \psi_{g'}(\bar{r}, \bar{\Omega}') d\bar{\Omega}' + Q_g(\bar{r}, \bar{\Omega}) \end{aligned} \quad (7)$$

for $g = 1, \dots, G$. In Eq. (7),

$$\psi_g(\bar{r}, \bar{\Omega}) = \int_{E_g}^{E_{g-1}} \psi(\bar{r}, \bar{\Omega}, E) dE$$

and

$$\sigma_g(\bar{r}) = \frac{\int_{E_g}^{E_{g-1}} \sigma(\bar{r}, E) \psi(\bar{r}, \bar{\Omega}, E) dE}{\psi_g(\bar{r}, \bar{\Omega})}$$

and

$$\begin{aligned} \sigma_{sg \rightarrow g}(\bar{r}, \bar{\Omega}' \rightarrow \bar{\Omega}) \\ = \frac{\int_{E_g}^{E_{g-1}} \int_{E_g'}^{E_{g'-1}} \sigma_s(\bar{r}, \bar{\Omega}' \rightarrow \bar{\Omega}, E' \rightarrow E) \psi(\bar{r}, \bar{\Omega}', E') dE' dE}{\psi_g(\bar{r}, \bar{\Omega}')} \end{aligned}$$

This set of equations can be solved for the set of flux functions, $\{\psi_g(\bar{r}, \bar{\Omega})\}$ $g = 1, \dots, G$. The set of equations is solved using an iterative procedure. The iterations involved are called outer iterations. This outer iteration procedure is different depending on whether a fixed source problem or an eigenvalue problem is being solved.

For a fixed source problem Eq. (7) can be rewritten as

$$\begin{aligned} \bar{\Omega} \cdot \nabla \psi_g(\bar{r}, \bar{\Omega}) + \sigma_g(\bar{r}) \psi_g(\bar{r}, \bar{\Omega}) \\ = \int \sigma_{sg \rightarrow g}(\bar{r}, \bar{\Omega}' \rightarrow \bar{\Omega}) \psi_g(\bar{r}, \bar{\Omega}') d\bar{\Omega}' + \hat{Q}_g(\bar{r}, \bar{\Omega}) \end{aligned} \quad (8)$$

where

$$\hat{Q}_g(\bar{r}, \bar{\Omega}) = Q_g(\bar{r}, \bar{\Omega}) + \int \sum_{\substack{g'=1 \\ g' \neq g}}^G \sigma_{sg' \rightarrow g}(\bar{r}, \bar{\Omega}' \rightarrow \bar{\Omega}) \psi_{g'}(\bar{r}, \bar{\Omega}') d\bar{\Omega}' \quad (9)$$

The iteration procedure is to start with the highest energy group and solve Eq. (8). To do this an initial set of fluxes, $\{\psi_g^{(0)}\}$ $g = 1, \dots, G$ is guessed. The set $\{\psi_g^{(0)}\}$ $g = 1, \dots, G$ is used to find $\hat{Q}_g^{(0)}(\bar{r}, \bar{\Omega})$ and then Eq. (8) is solved for $\psi_1^{(1)}(\bar{r}, \bar{\Omega})$. Next Eq. (8) is solved for $\psi_2^{(1)}(\bar{r}, \bar{\Omega})$ where the set $\{\psi_1^{(1)}\} \cup \{\psi_g^{(0)}\}$ $g = 3, \dots, G$ is used to find $\hat{Q}_1^{(0)}(\bar{r}, \bar{\Omega})$. This procedure continues until the entire set $\{\psi_g^{(1)}\}$ $g = 1, \dots, G$ has been found. When this is done then one outer iteration has been completed. So the outer iteration for a fixed source problem is

$$\begin{aligned} \bar{\Omega} \cdot \nabla \psi_g^{(k)}(\bar{r}, \bar{\Omega}) + \sigma_g(\bar{r}) \psi_g^{(k)}(\bar{r}, \bar{\Omega}) \\ = \int \sigma_{sg \rightarrow g}(\bar{r}, \bar{\Omega}' \rightarrow \bar{\Omega}) \psi_g^{(k)}(\bar{r}, \bar{\Omega}') d\Omega' + \hat{Q}_g^{(k-1)}(\bar{r}, \bar{\Omega}) \end{aligned} \quad (8a)$$

where

$$\begin{aligned} \hat{Q}_g^{(k-1)} = Q_g(\bar{r}, \bar{\Omega}) \\ + \int \left[\sum_{g'=1}^{g-1} \sigma_{sg' \rightarrow g}(\bar{r}, \bar{\Omega}' \rightarrow \bar{\Omega}) \psi_{g'}^{(k)}(\bar{r}, \bar{\Omega}') \right. \\ \left. + \sum_{g'=g+1}^G \sigma_{sg' \rightarrow g}(\bar{r}, \bar{\Omega}' \rightarrow \bar{\Omega}) \psi_{g'}^{(k-1)}(\bar{r}, \bar{\Omega}') \right] d\Omega' \end{aligned} \quad (9a)$$

and k is the iteration index.

For an eigenvalue problem Eq. (7) becomes

$$\bar{\Omega} \cdot \nabla \psi_g(\bar{r}, \bar{\Omega}) + \sigma_g(\bar{r}) \psi_g(\bar{r}, \bar{\Omega})$$

$$\begin{aligned}
&= \int \sum_{g=1}^G \sigma_{sg \rightarrow g}(\bar{r}, \bar{\Omega}' \rightarrow \bar{\Omega}) \psi_g(\bar{r}, \bar{\Omega}') d\bar{\Omega}' \\
&+ \frac{1}{k} \chi_g \int \sum_{g'=1}^G \nu \sigma_{fg'}(\bar{r}) \psi_{g'}(\bar{r}, \bar{\Omega}') d\bar{\Omega}' .
\end{aligned} \tag{10}$$

There are an infinite number of eigenvalues for this equation but there will always exist a real positive eigenvalue, $k_{\max}$, which is larger in magnitude than any other eigenvalue.⁵ Moreover, corresponding to $k_{\max}$ is an eigenfunction which is uniquely nonnegative. It is $k_{\max}$ and the corresponding eigenfunction that are being sought. The physical meaning of k is the ratio between the numbers of neutrons in successive generations, with the fission process being the separator between generations.

The iterative process which is used to find $k_{\max}$ and the corresponding ψ is to find a sequence of $k^{(m)}$ and corresponding $\psi^{(m)}$ (where m is the iteration index) such that $\lim_{m \rightarrow \infty} k^{(m)} = k$ and $\lim_{m \rightarrow \infty} \psi^{(m)} = \psi$.

Following along with the physical meaning of k , the equation used for $k^{(m)}$ is

$$\begin{aligned}
k^{(m)} &= \frac{\text{Fission neutrons produced by } \psi^{(m)}}{\text{Fission neutron source for } \psi^{(m)}} \\
&= \frac{\sum_{g=1}^G \chi_g \sum_{g'=1}^G \nu \sigma_{fg'}(\bar{r}) \psi_{g'}^{(m)}}{\sum_{g=1}^G \chi_g \sum_{g'=1}^G \nu \sigma_{fg'}(\bar{r}) \psi_{g'}^{(m-1)} k^{(m-1)}} .
\end{aligned} \tag{11}$$

The scattering source term is the first term on the right side of Eq. (10). It is broken into three parts as was done in the case of a fixed source problem.

The outer iteration for an eigenvalue problem is

$$\begin{aligned} \bar{\Omega} \cdot \nabla \psi_g^{(m)}(\bar{r}, \bar{\Omega}) + \sigma_g(\bar{r}) \psi_g^{(m)}(\bar{r}, \bar{\Omega}) \\ = \int \sigma_{sg \rightarrow g}(\bar{r}, \bar{\Omega}' \rightarrow \bar{\Omega}) \psi_g^{(m)}(\bar{r}, \bar{\Omega}') d\bar{\Omega}' + \hat{Q}_g^{(m-1)} \end{aligned} \quad (12a)$$

where

$$\begin{aligned} \hat{Q}_g^{(m-1)} = \int \sum_{g'=1}^{g-1} \sigma_{sg' \rightarrow g}(\bar{r}, \bar{\Omega}' \rightarrow \bar{\Omega}) \psi_{g'}^{(m)}(\bar{r}, \bar{\Omega}') \\ + \sum_{g'=g+1}^G \sigma_{sg' \rightarrow g}(\bar{r}, \bar{\Omega}' \rightarrow \bar{\Omega}) \psi_{g'}^{(m-1)}(\bar{r}, \bar{\Omega}') d\bar{\Omega}' \\ + \frac{1}{k^{(m-1)}} \chi_g \int \sum_{g'=1}^G v \sigma_{fg'}(\bar{r}) \psi_{g'}^{(m-1)}(\bar{r}, \bar{\Omega}') d\bar{\Omega}'. \end{aligned} \quad (12b)$$

So the first four steps of the iteration procedure for an eigenvalue problem are:

1. Guess $\psi_g^{(0)}(\bar{r}, \bar{\Omega})$ $g = 1, \dots, G$.
2. Guess $k^{(0)}$.
3. Solve Eq. (12a) for $\psi_g^{(1)}(\bar{r}, \bar{\Omega})$ $g = 1, \dots, G$.
4. Solve Eq. (11) for $k^{(1)}$.

Each outer iteration involves the solution of an equation of the form

$$\begin{aligned} \bar{\Omega} \cdot \nabla \psi(\bar{r}, \bar{\Omega}) + \sigma(\bar{r}) \psi(\bar{r}, \bar{\Omega}) \\ = \int_{\Omega} \sigma_s(\bar{r}, \bar{\Omega}' \rightarrow \bar{\Omega}) \psi(\bar{r}, \bar{\Omega}') d\bar{\Omega}' + Q(\bar{r}, \bar{\Omega}) \end{aligned} \quad (13)$$

for each energy group. This is identical to Eq. (8a) or Eq. (12a) except that the g subscripts have been dropped. The source, Q, in this case could either consist of an extraneous source and scattering from other groups (for a fixed source problem) or a fission source and scattering from other groups (for an eigenvalue problem). The scattering cross section, σ_s , is a within group scattering cross section.

Equation (13) is solved using an iteration process. The iterations used in solving Eq. (13) for each group are called inner iterations. The first step in this iterative process is to guess an initial flux, $\psi^{(0)}$. This flux is used on the right side of Eq. (13). Then the right side is known and the resulting differential equation is solved for ψ^1 . ψ^1 is then used on the right side of the equation and the procedure continues. These inner iterations may be described as

$$\begin{aligned} \bar{\Omega} \cdot \nabla \psi^k(\bar{r}, \bar{\Omega}) + \sigma(\bar{r}) \psi^k(\bar{r}, \bar{\Omega}) \\ = \int_{\Omega} \sigma_s(\bar{r}, \bar{\Omega}' \rightarrow \bar{\Omega}) \psi^{k-1}(\bar{r}, \bar{\Omega}') d\bar{\Omega}' + Q(\bar{r}, \bar{\Omega}) . \end{aligned} \quad (14)$$

B. Numerical Solution of the Inner Iteration in Slab Geometry

Some mathematical tools such as the spherical harmonics functions and Legendre polynomials will be described. Then these tools will be applied towards solving the inner iteration equation for one dimensional and two dimensional slab geometries. Finally difference equations will

be written for the special case of isotropic scattering and isotropic source in one dimensional and two dimensional slab geometry.

The Inner Iteration in Slab Geometry

Two special cases of the inner iteration as written in Eq. (14) will now be described.

The first case is the transport equation in one-dimensional slab geometry. The inner iteration for this case is

$$\begin{aligned} \mu \frac{\partial}{\partial x} \psi^k(x, \mu) + \sigma(x) \psi^k(x, \mu) &= \frac{1}{4\pi} \int_0^{2\pi} \int_{-1}^1 \sigma_s(x, \mu_0) \psi^{k-1}(x, \mu') d\mu' d\theta' \\ &+ Q(x, \mu) \end{aligned} \quad (15)$$

where μ_0 is defined in Eq. (5).

The second case to be considered is the transport equation in two-dimensional slab geometry. The inner iteration for this case is

$$\begin{aligned} \eta \frac{\partial}{\partial y} \psi^k(x, y, \mu, \theta) + \mu \frac{\partial}{\partial x} \psi^k(x, y, \mu, \theta) + \sigma(x, y) \psi^k(x, y, \mu, \theta) \\ = \frac{1}{4\pi} \int_0^{2\pi} \int_{-1}^1 \sigma_s(x, y, \mu_0) \psi^{k-1}(x, y, \mu', \theta') d\mu' d\theta' + Q(x, y, \mu, \theta) \end{aligned} \quad (16)$$

where $\eta = \sqrt{1 - \mu^2} \cos \theta$ and μ_0 is defined in Eq. (5).

In each case the discussion of the numerical method used will begin with a description of how the integrals in the scattering terms are evaluated. In order to evaluate them certain special functions are now described.

Legendre Polynomials and Spherical Harmonics

The Legendre polynomials constitute a familiar set of functions defined by the recursion relationship

$$P_{n+1}(\mu) = \frac{(2n+1)}{(n+1)} \mu P_n(\mu) - \frac{n}{(n+1)} P_{n-1}(\mu) \quad (17)$$

where $P_0(\mu) = 1$ and $P_1(\mu) = \mu$.¹ The associated Legendre polynomials are defined by

$$P_n^m(\mu) = (1 - \mu^2)^{\frac{m}{2}} \frac{d^m}{d\mu^m} P_n(\mu) \quad (18a)$$

and

$$P_n^{-m} = (-1)^m \frac{(n-m)!}{(n+m)!} P_n^m(\mu) \quad (18b)$$

where m is a positive integer such that $m \leq n$. The associated Legendre polynomials are used to define a complete set of functions in the angular variables μ and θ called the spherical harmonics.¹ They are defined by

$$Y_n^m(\mu, \theta) = \left[\frac{(2n+1)(n-m)!}{(n+m)!} \right]^{\frac{1}{2}} P_n^m(\mu) \exp(im\theta) \quad (19)$$

where n is a nonnegative integer and $-n \leq m \leq n$. The Y_n^m obey the orthogonality relationship

$$\frac{1}{4\pi} \int_0^{2\pi} \int_{-1}^1 \bar{Y}_r^s(\mu, \theta) Y_n^m(\mu, \theta) d\mu d\theta = \delta_{rn} \delta_{sm} \quad (20)$$

where $\bar{Y}_r^S$ is the complex conjugate of Y_r^S and δ_{rn} is the Kronecker delta.

Since

$$Y_n^0(\mu, \theta) = (2n + 1)^{\frac{1}{2}} P_n^0(\mu) = (2n + 1)^{\frac{1}{2}} P_n(\mu) ,$$

a similar relationship can be written involving Legendre polynomials. It is

$$\frac{(2n + 1)}{2} \int_{-1}^1 P_n(\mu) P_m(\mu) d\mu = \delta_{nm} .$$

Since the Y_n^m form a complete set, the function $\psi(x, y, \mu, \theta)$ can be expanded as

$$\psi(x, y, \mu, \theta) = \sum_{n=0}^{\infty} \sum_{m=-n}^n \phi_n^m(x, y) Y_n^m(\mu, \theta) \quad (21)$$

where, formally, the ϕ_n^m are defined as

$$\phi_n^m = \frac{1}{4\pi} \int_0^{2\pi} \int_{-1}^1 \psi(x, y, \mu, \theta) \bar{Y}_n^m(\mu, \theta) d\mu d\theta . \quad (22)$$

Similarly the function $\psi(x, \mu)$ can be expanded as

$$\psi(x, \mu) = \sum_{n=0}^{\infty} (2n + 1) \phi_n(x) P_n(\mu) \quad (23)$$

where

$$\phi_n(x) = \frac{1}{2} \int_{-1}^1 \psi(x, \mu) P_n(\mu) d\mu. \quad (24)$$

One other relationship that is used is one that relates the cosine of the scattering angle, μ_0 , with the direction vector before scattering, (μ', θ') , and the direction vector after scattering (μ, θ) . It is called the law of angular addition for Legendre polynomials. It is

$$P_n(\mu_0) = P_n(\mu') P_n(\mu) + 2 \sum_{m=1}^n \frac{(n-m)!}{(n+m)!} P_n^m(\mu') P_n^m(\mu) \cos m(\theta' - \theta). \quad (25)$$

The Scattering Integral in Slab Geometry

The above equations dealing with expansions of functions in terms of Legendre polynomials and spherical harmonics are now applied to the scattering integrals in one- and two-dimensional slab geometry.

The scattering integral in the case of one-dimensional slab geometry is

$$\frac{1}{4\pi} \int_0^{2\pi} \int_{-1}^1 \sigma_s(x, \mu_0) \psi^{k-1}(x, \mu') d\mu' d\theta'.$$

The scattering cross section and the flux are expanded in terms of Legendre polynomials yielding

$$\begin{aligned}
& \frac{1}{4\pi} \int_0^{2\pi} \int_{-1}^1 \sigma_s(x, \mu_0) \psi(x, \mu') d\mu' d\theta' \\
&= \frac{1}{4\pi} \int_0^{2\pi} \int_{-1}^1 \left[\sum_{\ell=0}^{\infty} (2\ell + 1) \sigma_{s\ell}(x) P_{\ell}(\mu_0) \right] \\
&\quad \times \left[\sum_{n=0}^{\infty} (2n + 1) \phi_n(x) P_n(\mu') \right] d\mu' d\theta' \tag{26}
\end{aligned}$$

where the superscript, $k-1$, has been dropped. Next Eq. (25) is substituted into Eq. (26) giving

$$\begin{aligned}
& \frac{1}{4\pi} \int_0^{2\pi} \int_{-1}^1 \left\{ \sum_{\ell=0}^{\infty} (2\ell + 1) \sigma_{s\ell}(x) \left[P_{\ell}(\mu') P_{\ell}(\mu) \right. \right. \\
&\quad \left. \left. + 2 \sum_{m=1}^{\ell} \frac{(\ell - m)!}{(\ell + m)!} P_{\ell}^m(\mu') P_{\ell}^m(\mu) \cos m(\theta' - \theta) \right] \right\} \\
&\quad \times \left[\sum_{n=0}^{\infty} (2n + 1) \phi_n(x) P_n(\mu') d\mu' d\theta' \right]
\end{aligned}$$

for the scattering integral.

Since

$$\frac{1}{2\pi} \int_0^{2\pi} \cos m(\theta' - \theta) d\theta' = 0,$$

when the integration over θ' is carried out the scattering integral becomes

$$\frac{1}{2} \int_{-1}^1 \left[\sum_{\ell=0}^{\infty} (2\ell + 1) \sigma_{s\ell}(x) P_{\ell}(\mu') P_{\ell}(\mu) \right] \\ \times \left[\sum_{n=0}^{\infty} (2n + 1) \phi_n(x) P_n(\mu') d\mu' \right].$$

Use of the orthogonality relationship yields

$$\sum_{\ell=0}^{\infty} (2\ell + 1) \sigma_{s\ell}(x) \phi_{\ell}(x) P_{\ell}(\mu) \quad (27)$$

which can be written as

$$\sum_{\ell=0}^{\infty} (2\ell + 1) \sigma_{s\ell}(x) P_{\ell}(\mu) \frac{1}{2} \int_{-1}^1 \psi(x, \xi) P_{\ell}(\xi) d\xi. \quad (28)$$

This is the form used in evaluating the scattering integral.

A similar process is now carried out on the scattering integral for the two-dimensional slab geometry case which is

$$\frac{1}{4\pi} \int_0^{2\pi} \int_{-1}^1 \sigma_s(x, y, \mu_0) \psi^{k-1}(x, y, \mu', \theta') d\mu' d\theta'. \quad (29)$$

The cross section is expanded in terms of Legendre polynomials and the flux is expanded in terms of spherical harmonics yielding

$$\frac{1}{4\pi} \int_0^{2\pi} \int_{-1}^1 \left[\sum_{\ell=0}^{\infty} (2\ell + 1) \sigma_{s\ell}(x, y) P_{\ell}(\mu_0) \right]$$

$$\times \left[\sum_{n=0}^{\infty} \sum_{m=-n}^n \phi_n^m(x, y) \gamma_n^m(\mu', \theta') \right] d\mu' d\theta'.$$

Next Eq. (25) and Eq. (19) are used to put the scattering integral in the form

$$\begin{aligned} & \frac{1}{4\pi} \int_0^{2\pi} \int_{-1}^1 \left[\sum_{\ell=0}^{\infty} (2\ell + 1) \sigma_{s\ell}(x, y) P_{\ell}(\mu') P_{\ell}(\mu) \right] \\ & \times \left[\sum_{n=0}^{\infty} \sum_{m=-n}^n \phi_n^m(x, y) \gamma_n^m(\mu', \theta') \right] d\mu' d\theta' \\ & + \frac{1}{4\pi} \int_0^{2\pi} \int_{-1}^1 \left\{ \left[\sum_{\ell=0}^{\infty} (2\ell + 1) \sigma_{s\ell}(x, y) \right] \right. \\ & \times \left[2 \sum_{k=1}^{\ell} \frac{(\ell - k)!}{(\ell + k)!} P_{\ell}^k(\mu') P_{\ell}^k(\mu) \cos k(\theta' - \theta) \right] \Big\} \\ & \times \left\{ \sum_{n=0}^{\infty} \sum_{m=-n}^n \phi_n^m \left[\frac{(2n + 1)(n - m)!}{(n + m)!} \right]^{\frac{1}{2}} P_n^m(\mu') \exp(im\theta') \right\} d\mu' d\theta'. \end{aligned}$$

The second integral in this expression is equal to zero because

$$\int_0^{2\pi} \cos k(\theta' - \theta) \exp(im\theta') d\theta' = 0$$

for any integers k and m . Using the fact that

$$(2\ell + 1)^{\frac{1}{2}} P_{\ell}(\mu') = \gamma_{\ell}^0(\mu', \theta') = \bar{\gamma}_{\ell}^0(\mu', \theta')$$

and the orthogonality relationship, Eq. (20); the first integral can be written

$$\sum_{\ell=0}^{\infty} (2\ell + 1)^{\frac{1}{2}} \sigma_{s\ell}(x,y) \phi_{\ell}^0(x,y) P_{\ell}(\mu) \quad (30)$$

where

$$\phi_{\ell}^0(x,y) = \frac{1}{4\pi} \int_0^{2\pi} \int_{-1}^1 \psi(x,y,\mu',\theta') P_{\ell}(\mu) d\mu' d\theta'.$$

So Eq. (27) and Eq. (30) are the desired forms of the scattering integral for one- and two-dimensional slab geometry. With this formulation the evaluation of the scattering term involves the evaluation of a series of integrals of fairly simple form. In practice the infinite series in Eq. (27) and Eq. (30) are truncated at $\ell = L$. A calculation which is performed using this truncation is called a P_L calculation. By way of illustration, the numerical method for calculating the zeroth term of the series in Eq. (27) and Eq. (30) is described under the heading, Finite Difference Equations with Isotropic Scattering and Source, beginning on page 22.

The Source Term Expansion

To be consistent with the scattering integral, the source term, Q , in Eq. (15) and Eq. (16) is expanded in terms of Legendre polynomials or spherical harmonics.

In the one-dimensional case of Eq. (15) the source is written as

$$Q(x, \mu) = \sum_{\ell=0}^{\infty} (2\ell + 1) Q_{\ell}(x) P_{\ell}(\mu) . \quad (31a)$$

In the two-dimensional case of Eq. (16) the source is written

$$Q(x, y, \mu, \theta) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} Q_{\ell}^m(x, y) Y_{\ell}^m(\mu, \theta) . \quad (31b)$$

Finite Difference Equations in Slab Geometry with Isotropic Scattering and Source

A special case of the transport equation is the one which involves isotropic scattering and an isotropic source. An isotropic function is one that is not dependent on an angular variable.

The inner iteration for one-dimensional slab geometry with isotropic scattering and source is

$$\mu \frac{\partial}{\partial x} \psi^k(x, \mu) + \sigma(x) \psi^k(x, \mu) = \sigma_s(x) \frac{1}{2} \int_{-1}^1 \psi^{k-1}(x, \mu') d\mu' + Q(x) . \quad (32)$$

Note that the scattering integral in this equation is exactly the same as the scattering integral that results from truncating Eq. (28) at $L = 0$. The source term here is the same as Eq. (31a) truncated at $L = 0$.

Now a description of how Eq. (32) is solved numerically is presented. The first step in writing the finite difference equation is to discretize the angular variable μ . A set of directions, $\{\mu_m\}_{m=1, \dots, M}$ is chosen.

Corresponding to each direction μ_m a quadrature weight w_m is chosen. Then the integral in Eq. (32) may be written as

$$\frac{1}{2} \int_{-1}^1 \psi(x, \mu) d\mu \approx \sum_{m=1}^M w_m \psi_m(x) \quad (33)$$

where $\psi_m(x) = \psi(x, \mu_m)$.⁶ In fact for any even M there is a unique set $\{\mu_m\}$ with corresponding $\{w_m\}$ such that the integration formula is exact for a polynomial in μ of order $2M - 1$. This set of quadrature parameters is called the Gauss quadrature set.⁵

The position variable, x , is discretized next. Suppose the length of the slab is R . Then the interval $[0, R]$ is partitioned into I cells. So a typical mesh cell is of width

$$\Delta x_i = x_{i + \frac{1}{2}} - x_{i - \frac{1}{2}}$$

where

$$x_{i + \frac{1}{2}} \text{ and } x_{i - \frac{1}{2}}$$

denote respectively the right and left boundaries of the i th mesh cell.

Then x_i denotes the center point of a mesh cell and is given by

$$x_i = \frac{1}{2} \left[x_{i - \frac{1}{2}} + x_{i + \frac{1}{2}} \right].$$

Thus $\psi_{im} = \psi_m(x_i)$. The partial derivative in Eq. (32) is differenced yielding

$$\frac{\mu_m}{\Delta x_i} \left(\psi_{mi}^k + \frac{1}{2} - \psi_{mi}^k - \frac{1}{2} \right) + \sigma_i \psi_{m,i}^k = \sigma_{si} \sum_{n=1}^M w_n \psi_{ni}^{k-1} + Q_i. \quad (34)$$

This is the finite difference form of the inner iteration in one dimensional slab geometry.

The inner iteration for the transport equation in two-dimensional slab geometry with isotropic scattering and source is

$$\begin{aligned} \eta \frac{\partial \psi^k}{\partial y}(x, y, \mu, \theta) + \mu \frac{\partial \psi^k}{\partial x}(x, y, \mu, \theta) + \sigma(x, y) \psi^k(x, y, \mu, \theta) \\ = \sigma_s(x, y) \int_0^{2\pi} \int_{-1}^1 \frac{1}{4\pi} \psi^{k-1}(x, y, \mu', \theta') d\mu' d\theta' + Q(x, y) \end{aligned} \quad (35)$$

where k is the iterate; and $\eta = \sqrt{1 - \mu^2} \cos \theta$. Note that the scattering integral in Eq. (35) is the same as the scattering integral that results from truncating Eq. (30) at $L = 0$. Also the source term in Eq. (35) is identical to the source term resulting from the truncation of Eq. (31b) at $L = 0$. The solution of the inner iteration for a problem in two dimensional slab geometry with isotropic scattering is equivalent to performing a P_0 calculation.

The difference equation used in solving Eq. (35) is now described. As in the one dimensional case a set of M directions is chosen. The Gauss quadrature set $\{\mu_m, \eta_m, w_m\}_{m=1, \dots, M}$ is used to approximate

the integral in Eq. (35) and the partial derivatives are approximated using finite difference methods yielding,

$$\begin{aligned} & \mu_m \frac{\psi_{mi}^k + \frac{1}{2} j - \psi_{mi}^k - \frac{1}{2} j}{\Delta x_i} + \eta_m \frac{\psi_{mij}^k + \frac{1}{2} - \psi_{mij}^k - \frac{1}{2}}{\Delta y_j} \\ & + \sigma_{ij} \psi_{mij} = \sigma_{sij} \sum_{n=1}^M w_n \psi_{nij}^{k-1} + Q_{mij}^3. \end{aligned} \quad (36)$$

This is the finite difference form of the inner iteration in two-dimensional slab geometry.

Differencing Methods and Boundary Conditions

The finite difference equations [Eq. (34) and Eq. (36)] are not of any use without boundary conditions and another set of equations relating the cell centered flux to the cell boundary fluxes.

In the one-dimensional case if there are I mesh cells on the interval $[0, R]$ then there are MI cell centered unknowns, $\{\psi_{mi}\}_{m=1, \dots, M}$ and $i = 1, \dots, I$, arising from Eq. (34). There are $M(I + 1)$ cell boundary unknowns, $\left\{\psi_{mi} + \frac{1}{2}\right\}_{m=1, \dots, M}$ and $i = 0, \dots, I$. So the total number of unknowns in a one-dimensional system is $(2I + 1)M$.

Equation (34) only gives rise to IM independent equations. This leaves a need for $(I + 1)M$ equations. Boundary conditions supply M of these equations. The other IM equations are supplied by difference equations which relate the flux in the center of any given cell with the flux on the boundaries of the cell.

Boundary conditions. Two types of boundary conditions were used in this work. One was the void boundary condition; the other was the reflected boundary condition.

The void boundary condition is stated as

$$\psi(0,\mu) = 0 \quad \text{for } \mu > 0$$

and

$$\psi(R,\mu) = 0 \quad \text{for } \mu < 0 .$$

One of the properties of a Gauss quadrature set is that for any μ_m in the set there exists $-\mu_m$ in the set.⁵ Thus the above boundary condition provides $M/2$ equations at each boundary.

The reflected boundary condition is stated as

$$\psi(0,\mu) = \psi(0,-\mu)$$

and

$$\psi(R,\mu) = \psi(R,-\mu)$$

These equations provide $M/2$ equations at each boundary.

Difference equations. Several different relationships are used to provide the IM remaining equations needed for solving the one-dimensional inner iteration in slab geometry.

The diamond difference equation is

$$\left(\psi_{mi}^k - \frac{1}{2} + \psi_{mi}^k + \frac{1}{2} \right) / 2 = \psi_{mi}^k . \quad (37)$$

It works well in many instances. However, with a coarse mesh negative fluxes are generated.⁵

A "negative fixup" method has been used when the diamond difference method generates negatives.⁷ It is called the linear step method. With this method

$$\psi_{mi}^k = \psi_{mi}^k + \frac{1}{2}$$

any time a negative flux is computed from Eq. (37).

Another difference equation is

$$\psi_{mi}^k = a \psi_{mi}^k - \frac{1}{2} + (1 - a) \psi_{mi}^k + \frac{1}{2} \quad (38)$$

where $1/2 < a < 1$. This is called the weighted difference formula.

A super weighted difference method has been developed by Rhoades and Engle.⁸ It differs from the weighted difference formula in the way that the weight, a , is chosen.

This completes the description of how the inner iteration is solved numerically for the one-dimensional transport equation in slab geometry.

The boundary conditions and difference formulas in two dimensions are completely analogous to the one-dimensional case.

III. STATEMENT OF THE THESIS PROBLEM

The problem that is solved in this thesis is now described.

The problem is to accelerate the convergence of the inner iterations of transport calculations performed by the computer code, DOT. This is done by developing subroutines that use the source correction scheme, implementing these routines into DOT, and finally, evaluating the effectiveness of these routines in accelerating the inner iterations in DOT. The measure of acceleration used in this work is the number of iterations required for convergence rather than the amount of CPU time required to run a problem.

The evaluation is performed by comparing results obtained with the source correction scheme with results obtained using the conventional rebalance method (which is in the current version of DOT) for several problems in one- and two-dimensional slab geometry.

IV. ACCELERATION OF INNER ITERATIONS

The theory of generalized rebalance has been used by Miller to accelerate the convergence of inner iterations for transport problems.⁶ An explanation of the general idea of rebalance will now be presented. Two rebalance schemes will be discussed. One is the conventional rebalance method (CRB). The other is the source correction scheme (SCS) as developed by Alcouffe.³ These methods will be described for the case of the inner iteration, Eq. (14), of the transport equation. Then the SCS will be described for one- and two-dimensional geometries and final difference equations will be presented.

A. The General Idea of Rebalance

The inner iteration for the transport equation was described above as

$$\begin{aligned} \bar{\Omega} \cdot \nabla \tilde{\psi}_g^k(\bar{r}, \bar{\Omega}) + \sigma_g(\bar{r}) \tilde{\psi}_g^k(\bar{r}, \bar{\Omega}) \\ = \int_{\bar{\Omega}'} \sigma_{sg \rightarrow g}(\bar{r}, \bar{\Omega}' \rightarrow \bar{\Omega}) \psi_g^{k-1}(\bar{r}, \bar{\Omega}') d\bar{\Omega}' + Q(\bar{r}, \bar{\Omega}) . \end{aligned} \quad (39a)$$

This equation is identical to Eq. (14) except that the g subscripts have been put back in and a tilde has been added to the fluxes on the left side of the equation. The symbol, $\tilde{\psi}$, represents a flux that is yet to be improved by a rebalance procedure.

The iteration procedure without rebalancing is described in the following steps:

1. $k = 1$.
2. Solve for $\tilde{\psi}_g^k$ knowing ψ_g^{k-1} using Eq. (39a).
3. If

$$\left| \frac{\tilde{\psi}_g^k - \psi_g^{k-1}}{\psi_g^{k-1}} \right| < \epsilon$$

for each point in the system then convergence has been obtained.

4. $k = k + 1$.
5. $\psi_g^{k-1} = \tilde{\psi}_g^{k-1}$.
6. Go to step (2).

Without rebalancing many transport problems converge slowly. Next the iteration procedure with rebalancing is described.

Of great importance in the rebalance procedure is the quantity

$$\int_{\Omega} \psi_g^{k-1}(\bar{r}, \bar{\Omega}') d\bar{\Omega}' .$$

It is called the scalar flux and will be represented by $\phi_g^{k-1}(\bar{r})$. In fact, from Eq. (22) it is seen that

$$\phi_g^{k-1}(\bar{r}) = \phi_{0g}^{0k-1}(\bar{r}) = \int_{\Omega} \psi_g^{k-1}(\bar{r}, \bar{\Omega}') \bar{Y}_0^0(\bar{\Omega}') d\bar{\Omega}' . \quad (40)$$

The iteration procedure with rebalancing is described in the following steps:

1. $k = 1$.
2. Solve for $\tilde{\psi}_g^k(\bar{r}, \bar{\Omega})$ knowing $\psi_g^{k-1}(\bar{r}, \bar{\Omega})$ using Eq. (39a).
3. Find an improved scalar flux, $\phi_g^k(\bar{r})$, using $\tilde{\psi}_g^k(\bar{r}, \bar{\Omega})$.
4. Find an improved directional flux, $\psi_g^k(\bar{r}, \bar{\Omega})$, using $\phi_g^k(\bar{r})$.
5. If

$$\left| \frac{\psi_g^k(\bar{r}, \bar{\Omega}) - \psi_g^{k-1}(\bar{r}, \bar{\Omega})}{\psi_g^{k-1}(\bar{r}, \bar{\Omega})} \right| < \epsilon$$

for each point of the system then convergence has been obtained.

6. $k = k + 1$.
7. Go to step (2).

The heart of the rebalance procedure is step (3) and step (4).

Three ways of performing step (3) and two ways of performing step (4) are described in this section. The name of each of these methods is in Table 1.

Table 1
Different Rebalance Methods

Step (3)	Step (4)
A. Alcouffe's flow term (SCS)	A. Scalar moment
B. Modified flow term (SCS)	B. All moments
C. Conventional rebalance	

One of the main computer codes in use at Oak Ridge National Laboratory for solving transport problems is called DOT. It uses a

sophisticated form of the conventional rebalance method for step (3) and the all moments method for step (4). Method A and Method B under step (3) in Table 1 are two different versions of the source correction scheme (SCS). Method A of performing step (4) is also unique to the SCS.

The SCS had not been used in the DOT code previously. The main purpose of this work was to incorporate the SCS method as promulgated by Miller and Alcouffe into the DOT code.^{6,3}

B. Three Methods of Finding $\phi_g^k(\bar{r})$ Based on a Knowledge of $\tilde{\psi}_g^k(\bar{r}, \bar{\Omega})$

In this subsection three methods of performing step (3) in the rebalance procedure are described.

The Conventional Rebalance Method

The method now being used in DOT is a sophisticated version of the conventional rebalance method. This is Method C of step (3) in Table 1.

The first step in deriving the CRB is to write the inner iteration of the transport equation for the case of isotropic scattering and source which is

$$\bar{\Omega} \cdot \nabla \tilde{\psi}_g^k(\bar{r}, \bar{\Omega}) + \sigma_g(\bar{r}) \tilde{\psi}_g^k(\bar{r}, \bar{\Omega}) = \sigma_{sg \rightarrow g}(\bar{r}) \phi_g^{k-1}(\bar{r}) + Q_g(\bar{r}) \quad (41)$$

This equation is then integrated over Ω yielding,

$$\nabla \cdot \int_{\Omega} \bar{\Omega} \tilde{\psi}_g^k(\bar{r}, \bar{\Omega}) d\Omega + \sigma_g(\bar{r}) \tilde{\phi}_g^k(\bar{r}) = \sigma_{sg \rightarrow g}(\bar{r}) \phi_g^{k-1}(\bar{r}) + Q_g(\bar{r}) . \quad (42)$$

Recall that $\sigma_g(\bar{r})$ represents the probability of a neutron in the g th energy group undergoing an interaction. The possible interactions are divided into two categories. One category of interactions is the category represented by $\sigma_{sg \rightarrow g}$. That is the probability of an interaction resulting only in a change of angle but not in a change of energy group. The other category consists of all other interactions which a particle could undergo. All of the interactions in this second category involve a removal of the neutron from the energy group g . Thus the probability of an interaction falling in the second category is represented by $\sigma_{Rg}(\bar{r})$ and

$$\sigma_{Rg}(\bar{r}) = \sigma_g(\bar{r}) - \sigma_{sg \rightarrow g}(\bar{r}) . \quad (43)$$

If it is assumed that at convergence $\tilde{\phi}_g^k(\bar{r}) = \phi_g^{k-1}(\bar{r})$ then Eq. (42) becomes

$$\nabla \cdot \tilde{J}_g(\bar{r}) + \sigma_{Rg}(\bar{r}) \tilde{\phi}_g^k(\bar{r}) = Q_g(\bar{r}) \quad (44)$$

where

$$\tilde{J}_g(\bar{r}) = \int_{\Omega} \tilde{\Omega} \tilde{\psi}_g^k(\bar{r}, \tilde{\Omega}) d\Omega .$$

$\tilde{J}_g(\bar{r})$ is called either the current or the flow term. A rebalance factor, $f_g^k(\bar{r})$, is introduced which is equal to the ratio of the improved scalar flux to the unimproved scalar flux. That is,

$$f_g^k(\bar{r}) = \phi_g^k(\bar{r}) / \tilde{\phi}_g^k(\bar{r}) . \quad (45)$$

The correction equation for the CRB method is

$$\nabla \cdot \left[f_g^k(\bar{r}) \tilde{J}(\bar{r}) \right] + \sigma_{Rg}(\bar{r}) f_g^k(\bar{r}) \tilde{\phi}_g^k(\bar{r}) = Q_g(\bar{r}) .^6 \quad (44a)$$

The conventional rebalance method proceeds in the following way. First Eq. (39a) is solved for $\tilde{\psi}_g^k(\bar{r}, \bar{\Omega})$. Then the correction equation (44a) is solved for $f_g^k(\bar{r})$. Then Eq. (45) is used to find the improved scalar flux, $\phi_g^k(\bar{r})$. Then the improved directional flux, $\psi_g^k(\bar{r}, \bar{\Omega})$, is found based on a knowledge of the improved scalar flux, $\phi_g^k(\bar{r})$, and one iteration is complete. The ways that $\psi_g^k(\bar{r}, \bar{\Omega})$ is found based on $\phi_g^k(\bar{r})$ are discussed in the next subsection which is entitled, "Finding $\psi_g^k(\bar{r}, \bar{\Omega})$ Based on $\phi_g^k(\bar{r})$."

Even though the correction equation was derived from the inner iteration with isotropic scattering and source, the same correction equation is used in the case of anisotropic scattering and source.

This completes the derivation of the CRB listed in Table 1, page 31, as Method C of step (3).

The SCS with the Alcouffe Flow Term

The next method described is the source correction scheme with the Alcouffe flow term.³ It is Method A of step (3) in Table 1. The SCS is a rebalance method which has only very recently been incorporated in the DOT code.

This method uses a correction equation to perform step (3) of the rebalance procedure, as did the CRB. The correction equation for the SCS is similar to Eq. (44).

The SCS correction equation is different from Eq. (44) in that the diffusion operator appears in the SCS correction equation. The diffusion operator is $-\nabla \cdot D_g(\bar{r}) \nabla$ where the diffusion coefficient,

$$D_g(\bar{r}) = 1/3[\sigma_g(\bar{r}) - \bar{\mu}_0 \sigma_{sg}(\bar{r})] . \quad (46)$$

The symbol, $\bar{\mu}_0$, is the cosine of the scattering angle averaged over all the isotopes present.¹ In the special case of isotropic scattering $\bar{\mu}_0 = 0$.

The correction equation for the SCS with the Alcouffe flow term is

$$\begin{aligned} & -\nabla \cdot D_g(\bar{r}) \nabla \phi_g^k(\bar{r}) + \sigma_{Rg}(\bar{r}) \phi_g^k(\bar{r}) \\ & = Q_g(\bar{r}) - \nabla \cdot \tilde{J}_g(r) - \nabla \cdot D_g(\bar{r}) \nabla \tilde{\phi}_g^k(\bar{r}) . \end{aligned} \quad (47)$$

This equation is used to perform step (3) of the rebalancing procedure.

The SCS with the Alcouffe flow term proceeds in the following way. First Eq. (39a) is solved for $\tilde{\psi}_g^k(\bar{r}, \bar{\Omega})$. Then the correction equation, Eq. (47) is solved for $\phi_g^k(\bar{r})$. Finally $\psi_g^k(\bar{r}, \bar{\Omega})$ is found based on $\phi_g^k(\bar{r})$ and one iteration is complete. The ways that $\psi_g^k(\bar{r}, \bar{\Omega})$ is found based on $\phi_g^k(\bar{r})$ are described in the next subsection.

Note that at convergence Eq. (47) collapses to Eq. (44). Thus if the SCS converges it converges to the CRB correction equation which is a form of the converged transport equation.

The reason this method is so appealing is the fact that if the right side of Eq. (47) is considered as a corrected source then Eq. (47) is the diffusion equation. This is why this method is called the source correction scheme.

This completes the description of Method A under step (3) in Table 1, page 31.

The SCS with the Modified Flow Term

The next method of performing step (3) is a version of the SCS which involves a novel form of the flow term, $\tilde{J}_g(\bar{r})$. The correction equation in this case is similar to the Alcouffe version of SCS. The only difference arises from solving Eq. (42) for

$$\nabla \cdot \int_{\Omega} \bar{\Omega} \tilde{\psi}_g^k(\bar{r}, \bar{\Omega}) d\Omega$$

and substituting into Eq. (47) yielding

$$\begin{aligned} & -\nabla \cdot D_g(\bar{r}) \nabla \phi_g^k(\bar{r}) + \sigma_{Rg}(\bar{r}) \phi_g^k(\bar{r}) \\ & = Q_g(\bar{r}) - \left[Q_g(\bar{r}) - \sigma_g(\bar{r}) \tilde{\phi}_g^k(\bar{r}) + \sigma_{sg \rightarrow g}(\bar{r}) \phi_g^{k-1}(\bar{r}) \right] \\ & \quad - \nabla \cdot D_g(\bar{r}) \nabla \tilde{\phi}_g^k(\bar{r}) \\ & = \sigma_{Rg}(\bar{r}) \tilde{\phi}_g^k(\bar{r}) - \sigma_{sg \rightarrow g}(\bar{r}) \left[\phi_g^{k-1}(\bar{r}) - \tilde{\phi}_g^k(\bar{r}) \right] \\ & \quad - \nabla \cdot D_g(\bar{r}) \nabla \tilde{\phi}_g^k(\bar{r}) \end{aligned} \tag{48}$$

which is the correction equation for the modified flow term version of the SCS. It is used to perform step (3) of the rebalance procedure.

So the SCS with the modified flow term proceeds in the following way. First Eq. (39a) is solved for $\tilde{\psi}_g^k(\bar{r}, \bar{\Omega})$. Then the correction equation, Eq. (48), is solved for $\phi_g^k(\bar{r})$. Finally $\psi_g^k(\bar{r}, \bar{\Omega})$ is found based on $\phi_g^k(\bar{r})$ and one iteration is complete. The ways that $\psi_g^k(\bar{r}, \bar{\Omega})$ is found based on $\phi_g^k(\bar{r})$ are described in the next subsection.

Note that at convergence Eq. (48) reduces to the identity, $0 = 0$.

This completes the derivation of Method B under step (3) in Table 1, page 31.

C. Finding $\psi_g^k(\bar{r}, \bar{\Omega})$ Based on $\phi_g^k(\bar{r})$

Two different methods are now discussed for performing step (4) of the rebalance procedure, that is, finding the improved directional flux, $\psi_g^k(\bar{r}, \bar{\Omega})$ based on the knowledge of the improved scalar flux, $\phi_g^k(\bar{r})$.

The directional flux can be expanded in terms of spherical harmonics as was seen above. Then the flux is

$$\psi_g(\bar{r}, \bar{\Omega}) = \sum_{n=0}^{\infty} \sum_{m=-n}^n \phi_{gn}^m(\bar{r}) Y_n^m(\bar{\Omega}) \quad (49a)$$

where

$$\phi_{gn}^m(\bar{r}) = \int_{\Omega} \psi_g(\bar{r}, \bar{\Omega}) Y_n^m(\bar{\Omega}) d\Omega. \quad (49b)$$

The two methods mentioned under step (4) in Table 1 are described next.

The Scalar Moment Method

This method was used by Miller to perform step (4) of the rebalance procedure.⁶ It is Method A of step (3) in Table 1, page 31. With this method the improved directional flux is found from the improved scalar flux using

$$\psi_g^k(\bar{r}, \bar{\Omega}) = \phi_{g0}^{0k}(\bar{r}) + \sum_{n=1}^{\infty} \sum_{\substack{m=-n \\ m \neq 0}}^n \tilde{\phi}_{gn}^{mk}(\bar{r}) Y_n^m(\bar{\Omega}) . \quad (50)$$

This method is called the scalar moment method because the improved directional flux is the sum of the improved scalar flux and the other flux moments which are unimproved. This method was not previously used in DOT.

The All Moments Method

The other method of performing step (4) of the rebalance procedure is called the all moments method. With this method all of the flux moments are improved by the same factor as the scalar flux. Let $f^k(\bar{r})$ be the rebalance factor defined as

$$f^k(\bar{r}) = \phi_{g0}^{0k}(\bar{r}) / \tilde{\phi}_{g0}^{0k}(\bar{r}) \quad (51)$$

Then the equation used to perform step (4) with the all moments method is

$$\psi_g^k(\bar{r}, \bar{\Omega}) = \sum_{n=1}^{\infty} \sum_{m=-n}^n f^k(\bar{r}) \tilde{\phi}_{gn}^{mk}(\bar{r}) Y_n^m(\bar{\Omega}) . \quad (52)$$

This is the description of Method B under step (4) in Table 1, page 31.

This concludes the discussion of each of the methods in Table 1.

D. The Source Correction Scheme in Slab Geometry

The SCS for the special cases of one- and two-dimensional slab geometry are now described.

The inner iteration for the transport equation in one-dimensional slab geometry is Eq. (15). The Alcouffe correction equation, Eq. (47), in one-dimensional slab geometry is

$$-\frac{d}{dx} \left[D(x) \frac{d\phi_0(x)}{dx} \right] + \sigma_R(x) \phi_0(x) = Q_0(x) - \frac{d}{dx} \left[D(x) \frac{d\tilde{\phi}_0(x)}{dx} \right] - \frac{d\tilde{\phi}_1}{dx} \quad (54)$$

where

$$\phi_0(x) = \frac{1}{2} \int_{-1}^1 \psi(x, \mu) d\mu ; \quad (55)$$

$$\phi_1(x) = \frac{1}{2} \int_{-1}^1 \mu \psi(x, \mu) d\mu ; \quad (56)$$

$$Q_0(x) = \frac{1}{2} \int_{-1}^1 Q(x, \mu) d\mu ; \quad (57)$$

and the k superscripts and g subscripts have been dropped.

The inner iteration for the transport equation in two-dimensional slab geometry is Eq. (16). The correction equation with the Alcouffe flow term for this case is

$$\begin{aligned}
 & - \frac{\partial}{\partial x} \left[D(x,y) \frac{\partial \phi_0(x,y)}{\partial x} \right] - \frac{\partial}{\partial y} \left[D(x,y) \frac{\partial \phi_0(x,y)}{\partial y} \right] \\
 & + \sigma_R(x,y) \phi_0(x,y) = Q_0(x,y) - \frac{\partial}{\partial x} \left[D(x,y) \frac{\partial \tilde{\phi}_0(x,y)}{\partial x} \right] \\
 & - \frac{\partial}{\partial y} \left[D(x,y) \frac{\partial \tilde{\phi}_0(x,y)}{\partial y} \right] - \frac{\partial}{\partial x} \tilde{\phi}_1(x,y) - \frac{\partial}{\partial y} \tilde{\phi}_2(x,y) \quad (58)
 \end{aligned}$$

where

$$\tilde{\phi}_0(x,y) = \frac{1}{4\pi} \int_0^{2\pi} \int_{-1}^1 \tilde{\psi}(x,y,\mu,\theta) d\mu d\theta ; \quad (59)$$

$$\tilde{\phi}_1(x,y) = \frac{1}{4\pi} \int_0^{2\pi} \int_{-1}^1 \mu \tilde{\psi}(x,y,\mu,\theta) d\mu d\theta ; \quad (60)$$

$$\tilde{\phi}_2(x,y) = \frac{1}{4\pi} \int_0^{2\pi} \int_{-1}^1 (\sqrt{1-\mu^2} \cos \theta) \tilde{\psi}(x,y,\mu,\theta) d\mu d\theta ; \quad (61)$$

and the k superscripts and g subscripts have been dropped.

The correction equation with the modified flow term in two-dimensional slab geometry is

$$- \frac{\partial}{\partial x} \left[D(x,y) \frac{\partial \phi_0(x,y)}{\partial x} \right] - \frac{\partial}{\partial y} \left[D(x,y) \frac{\partial \phi_0(x,y)}{\partial y} \right]$$

$$\begin{aligned}
& + \sigma_R(x,y) \phi_0(x,y) = \sigma_R(x,y) \tilde{\phi}_0(x,y) + \sigma_S(x,y) [\tilde{\phi}_0(x,y) - \phi_0^{k-1}(x,y)] \\
& - \frac{\partial}{\partial x} \left[D(x,y) \frac{\partial}{\partial x} \tilde{\phi}_0(x,y) \right] - \frac{\partial}{\partial y} \left[D(x,y) \frac{\partial}{\partial y} \tilde{\phi}_0(x,y) \right] . \quad (58a)
\end{aligned}$$

These are the forms of the correction equation for the SCS in slab geometry.

E. Numerical Solution of the Correction Equation in One-Dimensional Slab Geometry

In this section the numerical solution of the correction equation, [Eq. (54)], for one-dimensional slab geometry is discussed. The finite difference form of Eq. (54) is presented. This finite difference equation leads to a system of simultaneous linear equations. A description of how these equations are solved in the subroutine REBAL completes the section.

The Finite Difference Form of the One-Dimensional Correction Equation

The finite difference form of Eq. (54) is now derived. First the derivatives in brackets in the diffusion operators are written in difference form yielding

$$\begin{aligned}
& - \frac{d}{dx} \left\{ D(x) \left[\frac{\phi_{0i} + \frac{1}{2} - \phi_{0i} - \frac{1}{2}}{\Delta x_i} \right] \right\} + \sigma_R(x) \phi_0(x) \\
& = Q_0(x) - \frac{d}{dx} \left\{ D(x) \left[\frac{\tilde{\phi}_{0i} + \frac{1}{2} - \tilde{\phi}_{0i} - \frac{1}{2}}{\Delta x_i} \right] \right\} - \frac{d\tilde{\phi}_1(x)}{dx} . \quad (62)
\end{aligned}$$

Next, the remaining derivatives in the diffusion operators are differenced giving

$$\begin{aligned}
 & - \left\{ D_{i+1} \left[\frac{\left(\phi_{0i} + \frac{3}{2} - \phi_{0i} + \frac{1}{2} \right)}{\Delta x_{i+1}} \right] - D_i \left[\frac{\left(\phi_{0i} + \frac{1}{2} - \phi_{0i} - \frac{1}{2} \right)}{\Delta x_i} \right] \right\} / \Delta x_i \\
 & + \sigma_R(x) \phi_0(x) = Q_0(x) - d \frac{\tilde{\phi}_1}{dx}(x) \\
 & - \left\{ D_{i+1} \left[\frac{\tilde{\phi}_{0i} + \frac{3}{2} - \phi_{0i} + \frac{1}{2}}{\Delta x_i} \right] - D_i \left[\frac{\left(\phi_{0i} + \frac{1}{2} - \phi_{0i} - \frac{1}{2} \right)}{\Delta x_i} \right] \right\} / \Delta x_i .
 \end{aligned} \tag{63}$$

This leaves three terms yet to be discretized. The diffusion operator terms are evaluated at cell interfaces ($i - 1/2$, $i + 1/2$, $i + 3/2$). However the source and cross sections are known only for cell centered values of x . That is to say $\{\sigma_R(x_i), Q_0(x_i)\}$ $i = 1, \dots, I$ is known but

$$\left\{ \sigma_R\left(x_{i + \frac{1}{2}}\right), Q_0\left(x_{i + \frac{1}{2}}\right) \right\} i = 0, \dots, I$$

is not known. In order to discretize the source and cross section terms and have them evaluated at $i + 1/2$ the weighted average formulas,

$$[\sigma_R \phi]_{i + \frac{1}{2}} = (\sigma_{Ri} \phi_{0i} \Delta x_i + \sigma_{Ri+1} \Delta x_{i+1} \phi_{0i+1}) / 2 \Delta x_i \tag{64}$$

and

$$Q_{0i + \frac{1}{2}} = (Q_{0i} \Delta x_i + Q_{0i+1} \Delta x_{i+1}) / 2 \Delta x_i \tag{65}$$

are used. The derivative of $\tilde{\phi}_1$ is differenced so that it is evaluated at $i + 1/2$ yielding

$$\begin{aligned}
 & - \left\{ D_{i+1} \left[\frac{\phi_{0i} + \frac{3}{2} - \phi_{0i} + \frac{1}{2}}{\Delta x_{i+1}} \right] - D_i \left[\frac{\phi_{0i} + \frac{1}{2} - \phi_{0i} - \frac{1}{2}}{\Delta x_i} \right] \right\} / \Delta x_i \\
 & + (\sigma_{Ri} \phi_{0i} \Delta x_i + \sigma_{Ri+1} \Delta x_{i+1} \phi_{0i+1}) / 2 \Delta x_i \\
 & = (Q_{0i} \Delta x_i + Q_{0i+1} \Delta x_{i+1}) / 2 \Delta x_i - (\tilde{\phi}_{1i+1} - \tilde{\phi}_{1i}) / \Delta x_i \\
 & - \left\{ D_{i+1} \left[\frac{\tilde{\phi}_{0i} + \frac{3}{2} - \tilde{\phi}_{0i} + \frac{1}{2}}{\Delta x_{i+1}} \right] - D_i \left[\frac{\tilde{\phi}_{0i} + \frac{1}{2} - \tilde{\phi}_{0i} - \frac{1}{2}}{\Delta x_i} \right] \right\} / \Delta x_i
 \end{aligned} \tag{66}$$

which is the correction diffusion equation in one-dimensional slab geometry written in finite difference form.

Solution of the Finite Difference Form of the One-Dimensional Correction Equation

Next the actual procedure that was used to solve Eq. (66) is discussed. This task was performed by the subroutine REBAL which was run in conjunction with the transport code, DOT. This subsection is a description of how Eq. (66) was solved in REBAL.

The first item to describe is what information is supplied to REBAL by DOT and what information is returned to DOT when REBAL has completed its task.

DOT supplies to REBAL the following information:

1. $\{\tilde{\phi}_{0i}\} \quad i = 1, \dots, I$

2. $\{\tilde{\phi}_{1i}\} \quad i = 1, \dots, I.$
3. $\{Q_{0i}\} \quad i = 1, \dots, I.$
4. $\{\sigma_{si}\} \quad i = 1, \dots, I.$
5. $\{\sigma_i\} \quad i = 1, \dots, I.$
6. $\{\Delta x_i\} \quad i = 1, \dots, I.$

The information that is passed back to DOT is simply $\{\phi_{0i}\} \quad i = 1, \dots, I.$

It is seen from the right side of Eq. (66) that one of the first tasks of REBAL is to find the set $\{\tilde{\phi}_{0i + 1/2}\} \quad i = 0, \dots, I$ based on a knowledge of $\{\tilde{\phi}_{0i}\} \quad i = 0, \dots, I.$ A difference formula and a boundary condition are used to accomplish this task.

The different difference equations such as diamond, linear-step, weighted and superweighted were discussed above. In REBAL only the diamond difference formula

$$\tilde{\phi}_{0i + \frac{1}{2}} = 2\tilde{\phi}_{0i} - \tilde{\phi}_{0i - \frac{1}{2}} \quad (67)$$

was used. The entire set of cell boundary fluxes, $\{\tilde{\phi}_{0i + 1/2}\} \quad i = 0, \dots, I,$ can be found using Eq. (67) recursively provided that one member of the set is known since $\{\tilde{\phi}_{0i}\} \quad i = 1, \dots, I$ is known.

In fact a boundary condition will give two values in the set of cell boundary fluxes, namely $\tilde{\phi}_{0 \ 1/2}$ and $\tilde{\phi}_{0I + 1/2}.$ Two different boundary conditions were implemented in REBAL. They were the void boundary condition and the reflected boundary condition.

Two different ways of finding $\tilde{\phi}_{0 \ 1/2}$ and $\tilde{\phi}_{0I + 1/2}$ were used with a void boundary condition.

The first method is called the boundary ratio method. With this method the boundary values, $\tilde{\phi}_{0\ 1/2}$ and $\tilde{\phi}_{0I + 1/2}$ are not found in REBAL. They are found in DOT and then sent to REBAL. They are found in DOT by use of

$$\tilde{\phi}_{0p} = \sum_{m=1}^M \tilde{\psi}_{mp} w_m \quad (68)$$

for $p = 1/2$ and $p = I + 1/2$. So with the boundary ratio method the list of items sent to REBAL from DOT includes the two boundary values, $\tilde{\phi}_{0\ 1/2}$ and $\tilde{\phi}_{0I + 1/2}$.

The second method of incorporating the void boundary condition is called the extrapolation method. This method uses the fact that at a void boundary the scalar flux is known to decrease exponentially as in Fig. 2.

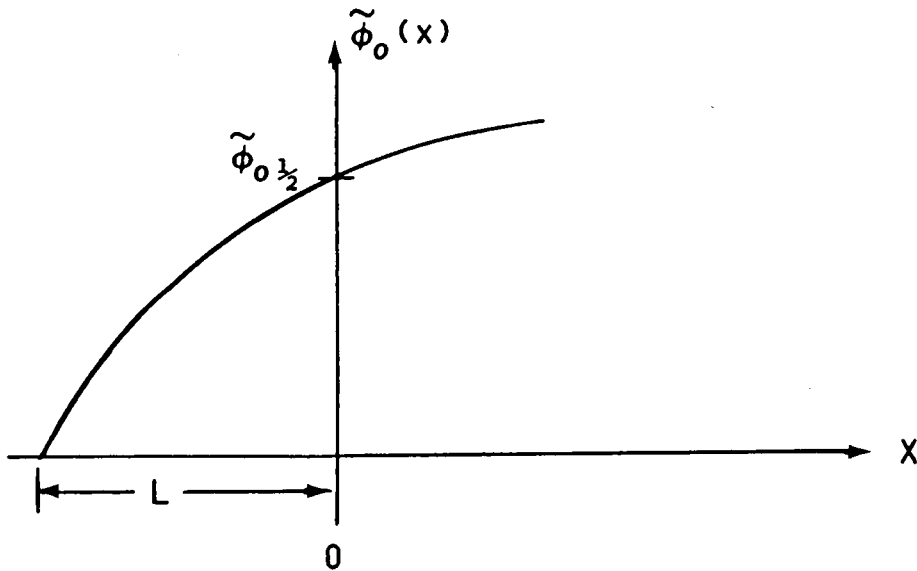


Fig. 2. Scalar Flux Dropoff at the Left Boundary.

The distance L in Fig. 2 at which the flux drops off to nearly zero has been found to be about $2.13 D_1$.³ This then gives the approximate slope of the flux at the boundary, giving rise to

$$\left. \frac{d}{dx} \tilde{\phi}_0(x) \right|_{x=0} \approx \frac{\tilde{\phi}_{0 \frac{1}{2}}}{2.13 D_1} \quad (69)$$

at the left boundary. In finite difference form Eq. (69) when it has been rearranged is

$$\tilde{\phi}_{0 \frac{1}{2}} = \frac{1}{1 + \frac{\Delta x_1}{2.13 D_1}} \tilde{\phi}_{0 \frac{3}{2}} \quad (70)$$

When the diamond difference formula [Eq. (67)] for $i = 1$ is substituted into Eq. (70) the result is

$$\tilde{\phi}_{0 \frac{1}{2}} = \frac{1}{1 + \frac{\Delta x_1}{4.26 D_1}} \tilde{\phi}_{01} \quad (71)$$

which is the formula used in REBAL to find $\tilde{\phi}_{0.1/2}$ from $\tilde{\phi}_{01}$ with the extrapolation method. A similar relationship can be derived for the right boundary which is how the right boundary value, $\phi_{I+1/2}$, is found in REBAL with the extrapolation method.

With the reflected boundary condition, REBAL receives the values $\tilde{\phi}_{0 \frac{1}{2}}$ and $\tilde{\phi}_{0I+1/2}$ from DOT. In DOT they are calculated using Eq. (68).

The way that the set $\{\tilde{\phi}_{0i} + 1/2\}$ $i = 0, \dots, I$ is found based on the set $\{\tilde{\phi}_{0i}\}$ $i = 1, \dots, I$ has now been described.

The next topic is the solution of the set of simultaneous linear equations represented by Eq. (66).

First Eq. (66) is written in "tridiagonal" form by substituting the diamond difference formula in the σ_R term and rearranging to get

$$\begin{aligned} & \left(\frac{\sigma_{Ri} \Delta x_i}{4} - \frac{D_i}{\Delta x_i} \right) \phi_{0i} - \frac{1}{2} + \left(\frac{D_{i+1}}{\Delta x_{i+1}} + \frac{D_i}{\Delta x_i} + \frac{\sigma_{Ri+1} \Delta x_{i+1} + \sigma_{Ri} \Delta x_i}{4} \right) \phi_{0i} + \frac{1}{2} \\ & + \left(\frac{\sigma_{Ri+1} \Delta x_{i+1}}{4} - \frac{D_{i+1}}{\Delta x_{i+1}} \right) \phi_{0i} + \frac{3}{2} = (\Delta x_{i+1} Q_{0i+1} + \Delta x_i Q_{0i})/2 \\ & - \frac{D_i}{\Delta x_i} \tilde{\phi}_{0i} - \frac{1}{2} + \left(\frac{D_{i+1}}{\Delta x_{i+1}} + \frac{D_i}{\Delta x_i} \right) \tilde{\phi}_{0i} + \frac{1}{2} - \frac{D_{i+1}}{\Delta x_{i+1}} \tilde{\phi}_{0i} + \frac{3}{2} \\ & + (\tilde{\phi}_{1i} - \tilde{\phi}_{1i+1}) . \end{aligned} \quad (72)$$

Two different sets of equations arise from Eq. (72) depending on whether a void boundary condition or a reflected boundary condition is imposed.

Suppose a void boundary condition is imposed on the left and the right. Then $I-1$ independent equations result from substituting $i = 1, \dots, I-1$ into Eq. (72). The right side of each of these equations is known. These $I-1$ equations contain $I+1$ unknowns, namely $\{\phi_{0i} + 1/2\}$ $i = 0, \dots, I$. The number of unknowns is reduced to $I-1$ through equations gotten from the boundary condition. The equations used depend on whether

the boundary ratio method or the extrapolation method is being used to approximate the void boundary.

If the boundary ratio method is used then the two extra equations are

$$\phi_{0 \frac{1}{2}} = \frac{\tilde{\phi}_{0 \frac{1}{2}}}{\tilde{\phi}_{0 \frac{3}{2}}} \phi_{0 \frac{3}{2}} \quad (73a)$$

and

$$\phi_{0I + \frac{1}{2}} = \frac{\tilde{\phi}_{0I + \frac{1}{2}}}{\tilde{\phi}_{0I - \frac{1}{2}}} \phi_{0I - \frac{1}{2}} \quad (73b)$$

If the extrapolation method is used then the two extra equations are

$$\phi_{0 \frac{1}{2}} = \frac{1}{\left(1 + \frac{\Delta x_1}{2.13 D_1}\right)} \phi_{0 \frac{3}{2}} \quad (74a)$$

and

$$\phi_{0I + \frac{1}{2}} = \frac{1}{\left(1 + \frac{\Delta x_I}{2.13 D_I}\right)} \phi_{0I - \frac{1}{2}} \quad (74b)$$

In either case the equations generated by substituting $i = 1$ and $i = I - 1$ into Eq. (72) can be written as

$$\begin{aligned}
& \left[(1 + C_L) \frac{\sigma_{R1} \Delta x_1}{4} + (1 - C_L) \frac{D_1}{\Delta x_1} + \frac{\sigma_{R2} \Delta x_2}{4} + \frac{D_2}{\Delta x_2} \right] \phi_{0 \frac{3}{2}} \\
& + \left[\frac{\sigma_{R2} \Delta x_2}{4} - \frac{D_2}{\Delta x_2} \right] \phi_{0 \frac{5}{2}} = (\Delta x_2 Q_{02} + \Delta x_1 Q_{01})/2 \\
& - \frac{D_1}{\Delta x_1} \tilde{\phi}_{0 \frac{1}{2}} + \left(\frac{D_2}{\Delta x_2} + \frac{D_1}{\Delta x_1} \right) \tilde{\phi}_{0 \frac{3}{2}} - \frac{D_2}{\Delta x_2} \tilde{\phi}_{0 \frac{5}{2}} + (\tilde{\phi}_{11} - \tilde{\phi}_{12}) \quad (75)
\end{aligned}$$

and

$$\begin{aligned}
& \left[(1 + C_R) \frac{\sigma_{RI} \Delta x_I}{4} + (1 - C_R) \frac{D_I}{\Delta x_I} + \frac{D_{I-1}}{\Delta x_{I-1}} + \frac{\sigma_{RI-1} \Delta x_{I-1}}{4} \right] \phi_{0I - \frac{1}{2}} \\
& + \left(\frac{\sigma_{RI-1} \Delta x_{I-1}}{4} - \frac{D_{I-1}}{\Delta x_{I-1}} \right) \phi_{0I - \frac{3}{2}} = (\Delta x_I Q_{0I} + \Delta x_{I-1} Q_{0I-1})/2 \\
& - \frac{D_{I-1}}{\Delta x_{I-1}} \tilde{\phi}_{0I + \frac{1}{2}} + \left(\frac{D_I}{\Delta x_I} + \frac{D_{I-1}}{\Delta x_{I-1}} \right) \tilde{\phi}_{I - \frac{1}{2}} - \frac{D_I}{\Delta x_I} \tilde{\phi}_{0I - \frac{3}{2}} \\
& + (\tilde{\phi}_{1I-1} - \tilde{\phi}_{1I}) \quad (76)
\end{aligned}$$

respectively. These two equations along with Eq. (72) for $i = 2, \dots, I-2$ make up a system of $I-1$ equations which when put in matrix form yield an $(I-1) \times (I-1)$ tridiagonal matrix equation. The constants C_L and C_R are obtained from either Eq. (73) or Eq. (74). For example in the case of a void boundary done with the extrapolation method

$$C_R = \frac{1}{\left(1 + \frac{\Delta x_I}{2.13 D_I}\right)} . \quad (77)$$

Now suppose that a problem is being solved that has a reflected boundary on the left and on the right. The reflected boundary can be stated as

$$\psi(x, \mu) = \psi(-x, -\mu) \quad (78)$$

at the left boundary and

$$\psi(R + x, \mu) = \psi(R - x, -\mu) \quad (79)$$

at the right boundary. Thus since

$$\phi_0(x) = \frac{1}{2} \int_{-1}^1 \psi(x, \mu) d\mu$$

and

$$\phi_1(x) = \frac{1}{2} \int_{-1}^1 \mu \psi(x, \mu) d\mu$$

the reflected boundary condition can be stated as

$$\phi_0(x) = \phi_0(-x) \quad (80a)$$

$$\phi_0(R + x) = \phi_0(R - x) \quad (80b)$$

and

$$\phi_1(x) = -\phi_1(-x) \quad (81a)$$

$$\phi_1(R+x) = -\phi_1(R-x) \quad (81b)$$

If Eq. (72) is written for $i = 0, \dots, I$ then one has a system of $I+1$ equations with the $I+3$ unknowns, $\{\phi_{0i-1/2}\}_{i=0, \dots, I+2}$. The boundary conditions eliminate the extra unknowns and the resulting equations are

$$\begin{aligned} & 2 \left(\frac{D_1}{\Delta x_1} - \frac{\sigma_{R1} \Delta x_1}{4} \right) \phi_{0 \frac{1}{2}} + 2 \left(\frac{\sigma_{R1} \Delta x_1}{4} - \frac{D_1}{\Delta x_1} \right) \phi_{0 \frac{3}{2}} \\ & = \Delta x_1 Q_1 + 2 \frac{D_1}{\Delta x_1} \tilde{\phi}_{0 \frac{1}{2}} - 2 \frac{D_1}{\Delta x_1} \tilde{\phi}_{0 \frac{3}{2}} - 2 \tilde{\phi}_{11} \end{aligned} \quad (82)$$

and

$$\begin{aligned} & 2 \left(\frac{\sigma_{RI} \Delta x_I}{4} - \frac{D_I}{\Delta x_I} \right) \phi_{0I - \frac{1}{2}} + 2 \left(\frac{D_I}{\Delta x_I} + \frac{\sigma_{RI} \Delta x_I}{4} \right) \phi_{0I + \frac{1}{2}} \\ & = \Delta x_I Q_{0I} - 2 \frac{D_I}{\Delta x_I} \tilde{\phi}_{I - \frac{1}{2}} + 2 \frac{D_I}{\Delta x_I} \tilde{\phi}_{0I + \frac{1}{2}} + 2 \tilde{\phi}_{1I} \end{aligned} \quad (83)$$

and Eq. (72) for $i = 1, \dots, I-1$. When put in matrix form this yields a tridiagonal $(I+1) \times (I+1)$ matrix equation.

In both the case of void boundaries and the case of reflected boundaries for the one-dimensional diffusion correction equation it has

been shown that the problem of solving the system of equations arising from Eq. (72) is equivalent to inverting a tridiagonal matrix. The subroutine REBAL calls a subroutine SOLVER which uses the Thomas algorithm to invert a tridiagonal matrix.⁹

Once the tridiagonal system has been solved then a set of improved cell boundary fluxes is known. In the case of void boundaries this set is $\{\phi_{0i + 1/2}\}$ $i = 1, \dots, I-1$. In the case of reflected boundaries this set is $\{\phi_{0i + 1/2}\}$ $i = 0, \dots, I$. The final task to be done by REBAL is to find the improved cell centered fluxes, $\{\phi_{0i}\}$ $i = 1, \dots, I$. The diamond difference formula

$$\phi_{0i} = \left(\phi_{0i - \frac{1}{2}} + \phi_{0i + \frac{1}{2}} \right)^{1/2} \quad (84)$$

for $i = 1, \dots, I$ is used to find the improved cell centered fluxes based on the improved boundary fluxes.

In the case of reflected boundaries Eq. (84) can be solved because the set $\{\phi_{0i + 1/2}\}$ $i = 0, \dots, I$ is known.

In the case of void boundaries the values $\phi_{0 1/2}$ and $\phi_{0I + 1/2}$ must be found before the cell centered fluxes ϕ_{01} and ϕ_{0I} can be found from Eq. (84). If the boundary ratio method is used then Eq. (73) is used to find $\phi_{0 1/2}$ and $\phi_{0I + 1/2}$. If the extrapolation method is used then Eq. (74) is used to find $\phi_{0 1/2}$ and $\phi_{0I + 1/2}$. Then Eq. (84) is used to find the cell centered improved fluxes.

This completes the discussion of how the finite difference form of the one-dimensional slab geometry diffusion correction equation is solved in the subroutine REBAL.

F. Numerical Solution of the Correction Equations in Two-Dimensional Slab Geometry

This section contains a discussion of the finite difference forms of the two correction equations [Eq. (58) and Eq. (58a)] in two dimensional slab geometry. Then a description of how the subroutine TWODIM solves these finite difference equations is given.

The Finite Difference Forms of the Two-Dimensional Correction Equations

In two dimensional slab geometry the transport equation is solved on a rectangular region. Let this region be denoted by $\{(x,y) \mid 0 \leq x \leq R \text{ and } 0 \leq y \leq H\}$. Then let the y variable be discretized into J intervals and the x variable into I intervals. Then the rectangular region in question is made up of IJ mesh cells of the form seen in Fig. 3.

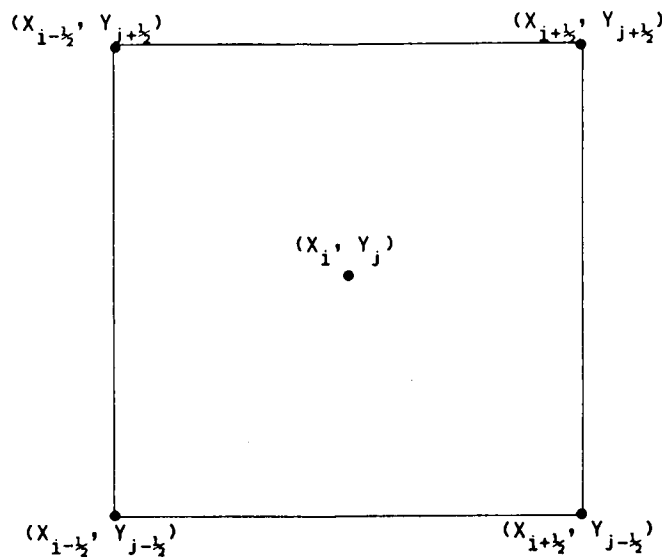


Fig. 3. A Typical Mesh Cell.

The correction equation with the Alcouffe flow term for the SCS in two-dimensional slab geometry is Eq. (58). A finite difference form of this equation was derived by Alcouffe.³ It is

$$\begin{aligned}
 & - \frac{(D_{i+1,j} \Delta y_j + D_{i+1,j+1} \Delta y_{j+1})}{2\Delta x_{i+1}} \left(\phi_{0i + \frac{3}{2}j + \frac{1}{2}} - \phi_{0i + \frac{1}{2}j + \frac{1}{2}} \right) \\
 & + \frac{(D_{ij} \Delta y_j + D_{ij+1} \Delta y_{j+1})}{2\Delta x_i} \left(\phi_{0i + \frac{1}{2}j + \frac{1}{2}} - \phi_{0i - \frac{1}{2}j + \frac{1}{2}} \right) \\
 & - \frac{(D_{ij+1} \Delta x_i + D_{i+1,j+1} \Delta x_{i+1})}{2\Delta y_{j+1}} \left(\phi_{0i + \frac{1}{2}j + \frac{3}{2}} - \phi_{0i + \frac{1}{2}j + \frac{1}{2}} \right) \\
 & + \frac{(D_{ij} \Delta x_i + D_{i+1,j} \Delta x_{i+1})}{2\Delta y_j} \left(\phi_{0i + \frac{1}{2}j + \frac{1}{2}} - \phi_{0i + \frac{1}{2}j - \frac{1}{2}} \right) \\
 & + \frac{1}{4} \left\{ (\sigma_{Rij} V_{ij} \tilde{\phi}_{0ij} + \sigma_{Ri+1j} V_{i+1j} \tilde{\phi}_{0i+1j} + \sigma_{Rij+1} V_{ij+1} \tilde{\phi}_{0ij+1} \right. \\
 & \quad \left. + \sigma_{Ri+1,j+1} V_{i+1,j+1} \tilde{\phi}_{0i+1,j+1}) / \tilde{\phi}_{0i + \frac{1}{2}j + \frac{1}{2}} \right\} \phi_{0i + \frac{1}{2}j + \frac{1}{2}} \\
 & = \frac{1}{4} (Q_{0ij} V_{ij} + Q_{0i+1j} V_{i+1j} + Q_{0ij+1} V_{ij+1} + Q_{0i+1,j+1} V_{i+1,j+1}) \\
 & - \frac{(D_{i+1,j} \Delta y_j + D_{i+1,j+1} \Delta y_{j+1})}{2\Delta x_{i+1}} \left(\tilde{\phi}_{0i + \frac{3}{2}j + \frac{1}{2}} - \tilde{\phi}_{0i + \frac{1}{2}j + \frac{1}{2}} \right) \\
 & + \frac{(D_{ij} \Delta y_j + D_{ij+1} \Delta y_{j+1})}{2\Delta x_i} \left(\tilde{\phi}_{0i + \frac{1}{2}j + \frac{1}{2}} - \tilde{\phi}_{0i - \frac{1}{2}j + \frac{1}{2}} \right) \\
 & - \frac{(D_{ij+1} \Delta x_i + D_{i+1,j+1} \Delta x_{i+1})}{2\Delta y_{j+1}} \left(\tilde{\phi}_{0i + \frac{1}{2}j + \frac{3}{2}} - \tilde{\phi}_{0i + \frac{1}{2}j + \frac{1}{2}} \right)
 \end{aligned}$$

$$\begin{aligned}
& + \frac{(D_{ij}\Delta x_i + D_{i+1j}\Delta x_{i+1})}{2\Delta y_j} \left(\tilde{\phi}_{0i + \frac{1}{2}j + \frac{1}{2}} - \tilde{\phi}_{0i + \frac{1}{2}j - \frac{1}{2}} \right) \\
& - \left[\frac{(\tilde{\phi}_{1i+1j}\Delta y_j + \tilde{\phi}_{1i+1j+1}\Delta y_{j+1})}{2} - \frac{(\tilde{\phi}_{1ij}\Delta y_j + \tilde{\phi}_{1ij+1}\Delta y_{j+1})}{2} \right] \\
& - \left[\frac{(\tilde{\phi}_{2ij+1}\Delta x_i + \tilde{\phi}_{2i+1j+1}\Delta x_{i+1})}{2} - \frac{(\tilde{\phi}_{2ij}\Delta x_i + \tilde{\phi}_{2i+1j}\Delta x_{i+1})}{2} \right]
\end{aligned} \tag{85}$$

where $V_{ij} = \Delta x_i \Delta y_j$.

Next the correction equation with the modified flow term in two-dimensional slab geometry [Eq. (58a)] is written in finite difference form. First, let all the terms on the left side of Eq. (85) containing a D be represented by $(D\phi)_{i + 1/2 j + 1/2}$. Similarly let all the terms containing the diffusion coefficient on the right side be represented by $(D\tilde{\phi}_0)_{i + 1/2 j + 1/2}$. Let the removal term (the sum of all terms containing σ_R) be represented by $(\sigma_R\phi_0)_{i + 1/2 j + 1/2}$ and let the source term (the sum of all terms containing a Q) be represented by $Q_{i + 1/2 j + 1/2}$. Then Eq. (85) with the modified flow term rather than the Alcouffe flow term is

$$\begin{aligned}
& (D\phi_0)_{i + \frac{1}{2}j + \frac{1}{2}} + (\sigma_R\phi_0)_{i + \frac{1}{2}j + \frac{1}{2}} \\
& = (D\tilde{\phi}_0)_{i + \frac{1}{2}j + \frac{1}{2}} + \left[\sigma_s (\tilde{\phi}_0 - \phi_0^{k-1}) + \sigma_R \tilde{\phi}_0 \right]_{i + \frac{1}{2}j + \frac{1}{2}}
\end{aligned} \tag{86}$$

where

$$\begin{aligned}
 & \left[\sigma_s (\tilde{\phi}_0 - \phi_0^{k-1}) + \sigma_R \tilde{\phi}_0 \right]_{i + \frac{1}{2}j + \frac{1}{2}} \\
 &= \frac{1}{4} \left\{ \left[\sigma_{sij} (\tilde{\phi}_{0ij} - \phi_{0ij}^{k-1}) + \sigma_{Rij} \tilde{\phi}_{0ij} \right] v_{ij} \right. \\
 &+ \left[\sigma_{si+1j} (\tilde{\phi}_{0i+1j} - \phi_{0i+1j}^{k-1}) + \sigma_{Ri+1j} \tilde{\phi}_{0i+1j} \right] v_{i+1j} \\
 &+ \left[\sigma_{sij+1} (\tilde{\phi}_{0ij+1} - \phi_{0ij+1}^{k-1}) + \sigma_{Rij+1} \tilde{\phi}_{0ij+1} \right] v_{ij+1} \\
 &+ \left. \left[\sigma_{si+1j+1} (\tilde{\phi}_{0i+1j+1} - \phi_{0i+1j+1}^{k-1}) + \sigma_{Ri+1j+1} \tilde{\phi}_{0i+1j+1} \right] v_{i+1j+1} \right\} \\
 & \hspace{15em} (87)
 \end{aligned}$$

and $\phi^{k-1}(x,y)$ is the improved flux that was computed one inner iteration previous to the one currently being rebalanced by Eq. (86). That is to say, each " ϕ " in Eq. (86) and Eq. (87) that has no superscript could be written with the superscript k .

This completes the description of the two different finite difference forms of the correction diffusion equation for two-dimensional slab geometry.

Solution of the Finite Difference Equations in the Subroutine TWODIM

This subsection contains an explanation of how the finite difference equations [Eq. (86) and Eq. (85)] are solved in the subroutine TWODIM which is run in conjunction with DOT. TWODIM is capable of running only problems with void boundary conditions.

The first item to describe is exactly what information is sent to TWODIM from DOT and what gets sent back from TWODIM to DOT. DOT provides TWODIM with the following:

1. $\{\tilde{\phi}_{0ij}\}$ $i = 1, \dots, I$ and $j = 1, \dots, J$.
2. $\{\tilde{\phi}_{1ij}\}$ $i = 1, \dots, I$ and $j = 1, \dots, J$.
3. $\{\tilde{\phi}_{2ij}\}$ $i = 1, \dots, I$ and $j = 1, \dots, J$.
4. $\{\tilde{\phi}_{1/2j}, \tilde{\phi}_{1I+1/2j}\}$ $j = 1, \dots, J$.
5. $\{\tilde{\phi}_{2i/2}, \tilde{\phi}_{2iJ+1/2}\}$ $i = 1, \dots, I$.
6. $\{\sigma_{Rij}, D_{ij}\}$ $i = 1, \dots, I$ and $j = 1, \dots, J$.
7. $\{\Delta x_i\}$ $i = 1, \dots, I$ and $\{\Delta y_j\}$ $j = 1, \dots, J$.
8. $\left\{ \left[\sigma_{sij}(\tilde{\phi}_{0ij} - \phi_{0ij}^{k-1}) + \sigma_{Rij}\tilde{\phi}_{0ij} \right] v_{ij} \right\}$ $i = 1, \dots, I$ and $j = 1, \dots, J$.

The information that is passed back to DOT by TWODIM is $\{f_{ij}\}$ $i = 1, \dots, I$ and $j = 1, \dots, J$ where $f_{ij} = \phi_{0ij}/\tilde{\phi}_{0ij}$ for $i = 1, \dots, I$ and $j = 1, \dots, J$.

The first task performed by TWODIM is to find the cell corner values,

$$\left\{ \tilde{\phi}_{0i + \frac{1}{2}j + \frac{1}{2}} \right\}_{\substack{i = 0, \dots, I \\ j = 0, \dots, J}},$$

based on the cell centered flux values,

$$\left\{ \tilde{\phi}_{0ij} \right\}_{\substack{i = 1, \dots, I \\ j = 1, \dots, J}}.$$

This is done for the interior cell corner fluxes with linear interpolation using

$$\tilde{\phi}_{0i + \frac{1}{2}j + \frac{1}{2}} = \frac{1}{4} (\tilde{\phi}_{0ij} + \tilde{\phi}_{0i+1,j} + \tilde{\phi}_{0ij+1} + \tilde{\phi}_{0i+1,j+1}) \quad (89)$$

for $i = 1, \dots, I-1$ and $j = 1, \dots, J-1$. The boundary cell corner fluxes (that is $\{\tilde{\phi}_{0 \frac{1}{2}j + \frac{1}{2}}, \tilde{\phi}_{0I + \frac{1}{2}j + \frac{1}{2}}\}_{j=1, \dots, J-1}$ and $\{\tilde{\phi}_{0i + \frac{1}{2} \frac{1}{2}}, \tilde{\phi}_{0i + \frac{1}{2}, J + \frac{1}{2}}\}_{i=1, \dots, I-1}$) are found using an equation from diffusion theory called Fick's law.² It is

$$\tilde{J}(\vec{r}) = -D(r)\nabla\tilde{\phi}_0(\vec{r}) . \quad (90)$$

Fick's law can be applied to the two-dimensional slab geometry boundary flows as

$$-D(b,y) \left. \frac{\partial \tilde{\phi}_0(x,y)}{\partial x} \right|_{x=b} = \tilde{\phi}_1(b,y) \quad (91)$$

for $b = 0$ and $b = R$ and

$$-D(x,b) \left. \frac{\partial \tilde{\phi}_0(x,y)}{\partial y} \right|_{y=b} = \tilde{\phi}_2(x,b) \quad (92)$$

for $b = 0$ and $b = H$.

In finite difference form Eq. (91) and Eq. (92) give rise to

$$\tilde{\phi}_{0 \frac{1}{2}j + \frac{1}{2}} = \tilde{\phi}_{0 \frac{3}{2}j + \frac{1}{2}} + \frac{\Delta x_1}{D_{1j}} \tilde{\phi}_{1 \frac{1}{2}j + \frac{1}{2}} \quad (93a)$$

for $j = 1, \dots, J-1$ and

$$\tilde{\phi}_{0I + \frac{1}{2}j + \frac{1}{2}} = \tilde{\phi}_{0I - \frac{1}{2}j + \frac{1}{2}} - \frac{\Delta x_I}{D_{Ij}} \tilde{\phi}_{1I + \frac{1}{2}j + \frac{1}{2}} \quad (93b)$$

for $j = 1, \dots, J-1$ and

$$\tilde{\phi}_{0i + \frac{1}{2}\frac{1}{2}} = \tilde{\phi}_{0i + \frac{1}{2}\frac{3}{2}} + \frac{\Delta y_1}{D_{i1}} \tilde{\phi}_{2i + \frac{1}{2}\frac{1}{2}} \quad (93c)$$

for $i = 1, \dots, I-1$ and

$$\tilde{\phi}_{0i + \frac{1}{2}J + \frac{1}{2}} = \tilde{\phi}_{0i + \frac{1}{2}J - \frac{1}{2}} - \frac{\Delta y_J}{D_{iJ}} \tilde{\phi}_{2i + \frac{1}{2}J + \frac{1}{2}} \quad (93d)$$

for $i = 1, \dots, I-1$. DOT supplies the values $\{\tilde{\phi}_{1\frac{1}{2}j}, \tilde{\phi}_{1I + \frac{1}{2}j}\}$
 $j = 1, \dots, J$ and $\{\tilde{\phi}_{2i\frac{1}{2}}, \tilde{\phi}_{2iJ + \frac{1}{2}}\}$ $i = 1, \dots, I$ which suffice to
 give the right side of Eq. (93 a-d) when the interpolation formulas

$$\tilde{\phi}_{1\frac{1}{2}j + \frac{1}{2}} = \frac{1}{2} \left(\tilde{\phi}_{1\frac{1}{2}j} + \tilde{\phi}_{1\frac{1}{2}j+1} \right) \quad (94a)$$

for $j = 1, \dots, J-1$ and

$$\tilde{\phi}_{1I + \frac{1}{2}j + \frac{1}{2}} = \frac{1}{2} \left(\tilde{\phi}_{1I + \frac{1}{2}j} + \tilde{\phi}_{1I + \frac{1}{2}j+1} \right) \quad (94b)$$

for $j = 1, \dots, J-1$ and

$$\tilde{\phi}_{2i + \frac{1}{2} \frac{1}{2}} = \frac{1}{2} \left(\tilde{\phi}_{2i \frac{1}{2}} + \tilde{\phi}_{2i+1 \frac{1}{2}} \right) \quad (94c)$$

for $i = 1, \dots, I-1$ and

$$\tilde{\phi}_{2i + \frac{1}{2} J + \frac{1}{2}} = \frac{1}{2} \left(\tilde{\phi}_{2iJ + \frac{1}{2}} + \tilde{\phi}_{2i+1 J + \frac{1}{2}} \right) \quad (94d)$$

for $i = 1, \dots, I-1$ are used. The unimproved flux at the corners of the region are found using what is called the planar method. With this method the flux at the corner of the region is assumed to be in a plane formed by the values of the flux at the other three corners of its mesh cell. For example, the flux at the lower left corner of the rectangular region is found using

$$\tilde{\phi}_{0 \frac{1}{2} \frac{1}{2}} = \tilde{\phi}_{0 \frac{1}{2} \frac{3}{2}} + \tilde{\phi}_{0 \frac{3}{2} \frac{1}{2}} - \tilde{\phi}_{0 \frac{3}{2} \frac{3}{2}}. \quad (95)$$

After the task of finding the cell corner fluxes has been completed it is seen that the entire right side of the finite difference equation is known. Thus either Eq. (85) or Eq. (86) can be written for $i = 1, \dots, I-1$ and $j = 1, \dots, J-1$ yielding a system of $(I-1)(J-1)$ equations with $(I+1)(J+1)$ unknowns, namely

$$\left\{ \phi_{0i + \frac{1}{2} j + \frac{1}{2}} \right\}_{\substack{i = 0, \dots, I \\ j = 0, \dots, J}}.$$

To reduce the number of unknowns down to the number of equations a boundary ratio method is used. Along the left boundary, for example, this amounts to introducing the equations

$$\phi_{0 \frac{1}{2} j + \frac{1}{2}} = \left(\tilde{\phi}_{0 \frac{1}{2} j + \frac{1}{2}} / \tilde{\phi}_{0 \frac{3}{2} j + \frac{1}{2}} \right) \phi_{0 \frac{3}{2} j + \frac{1}{2}} \quad (96)$$

for $j = 1, \dots, J-1$. This method, at the lower left corner of the region, introduces the equation

$$\phi_{\frac{1}{2} \frac{1}{2}} = \left(\tilde{\phi}_{\frac{1}{2} \frac{1}{2}} / \tilde{\phi}_{\frac{3}{2} \frac{3}{2}} \right) \phi_{\frac{3}{2} \frac{3}{2}}. \quad (97)$$

Other similar equations can be written for the three other boundaries and the three other corners. When these equations are substituted into the $(I-1)(J-1)$ equations arising from either Eq. (85) or Eq. (86) then a system of linear independent equations results. This system when written in matrix form can be solved by inverting a five stripe matrix.

TWODIM calls a subroutine, WWESOL, which was written by W. W. Engle and R. L. Childs.⁴ It was modified slightly to solve a general $n \times n$ five stripe matrix.

So after WWESOL has solved the five stripe matrix the improved flux values

$$\left\{ \phi_{0i + \frac{1}{2} j + \frac{1}{2}} \right\}_{\substack{i = 1, \dots, I-1 \\ j = 1, \dots, J-1}}$$

are known. Next the boundary ratio equations such as Eq. (96) and Eq. (97) are used to obtain the boundary cell corner fluxes,

$$\left\{ \phi_{0, \frac{1}{2}j + \frac{1}{2}}, \phi_{0I + \frac{1}{2}j + \frac{1}{2}} \right\}_{j = 0, \dots, J}$$

and

$$\left\{ \phi_{0i + \frac{1}{2}, \frac{1}{2}}, \phi_{0i + \frac{1}{2}, J + \frac{1}{2}} \right\}_{i = 0, \dots, I}.$$

Finally the cell centered rebalance factors are found using

$$f_{ij} = \frac{1}{4} \left(\frac{\phi_{0i - \frac{1}{2}, j - \frac{1}{2}}}{\tilde{\phi}_{0i - \frac{1}{2}, j - \frac{1}{2}}} + \frac{\phi_{0i + \frac{1}{2}, j - \frac{1}{2}}}{\tilde{\phi}_{0i + \frac{1}{2}, j - \frac{1}{2}}} + \frac{\phi_{0i - \frac{1}{2}, j + \frac{1}{2}}}{\tilde{\phi}_{0i - \frac{1}{2}, j + \frac{1}{2}}} + \frac{\phi_{0i + \frac{1}{2}, j + \frac{1}{2}}}{\tilde{\phi}_{0i + \frac{1}{2}, j + \frac{1}{2}}} \right) \quad (98)$$

for $i = 1, \dots, I$ and $j = 1, \dots, J$.

This completes the description of how TWODIM solves the finite difference form of the diffusion correction equation in two-dimensional slab geometry. This also concludes the discussion of the acceleration of the inner iterations through rebalancing.

V. NUMERICAL RESULTS AND COMPARISONS

In this section a comparison is made between the different versions of the SCS method that have been discussed in the previous section. Also a comparison is made between the effectiveness of the SCS and the effectiveness of the DOT conventional rebalance.

In the first subsection results from one-dimensional problems are given. Problems run by Miller at Los Alamos were run using DOT conventional rebalance and then with the SCS.⁶ Comparisons are made between the boundary ratio method and the extrapolation method which are two methods of incorporating a void boundary condition.

In the second subsection results from two-dimensional problems are presented. Two methods of approximating the flow term are the Alcouffe flow term as in Eq. (85) and the modified flow term as in Eq. (86). These two methods are compared for several problems.

Two methods were described in Sect. IV-C for finding $\psi(\bar{r}, \bar{\Omega})$ based on $\phi(\bar{r})$. They were the scalar moment method as described in Eq. (50) and the all moments method as described in Eq. (51). A comparison of these two methods is given.

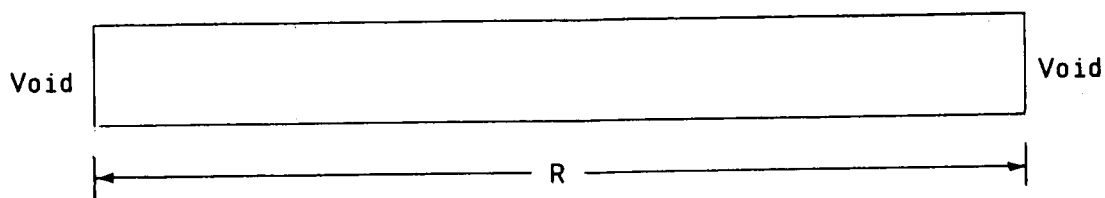
Another factor that seems to be crucial to the convergence rate of a problem is the dominance ratio. It is defined to be the ratio, $\sigma_{s0}(\bar{r})/\sigma(\bar{r})$. A study was made of how the dominance ratio effects convergence.

Lastly, a realistic two-dimensional problem was run using the DOT conventional rebalance as compared with the SCS.

A. Results in One-Dimensional Slab Geometry

All of the problems in this subsection were solved using the DOT-IV code with the subroutine REBAL. All of the problems are in one-dimensional slab geometry.

Miller published some results for one-dimensional problems.⁶ These problems are described in Table 2. All the problems were run using



diamond differencing with void boundaries. The slab thickness is denoted by R . A constant fixed source is distributed through all the mesh intervals.

Table 2
Description of Miller's Problems

Problem	σ in cm^{-1}	σ_{SO} in cm^{-1}	Δx in cm	R in cm
M1	1	1	1	30
M2	2	2	1	30
M3	1	1	1	60
M4	1	1	2	60
M5	3	2	1	30
M6	4	2	1	30
M7	1	0.75	1	30

The results of running these problems with DOT conventional rebalance, the boundary ratio SCS and the extrapolation SCS along with Miller's results are given in Table 3. The results from the extrapolation method agree well with Miller's results. The most obvious conclusion to be drawn here is that the SCS method converges faster than conventional DOT rebalance. Comparison of problem M1 with problem M7 shows that all of the methods converge faster for a problem with lower dominance ratio.

Table 3
Comparison of the Source Correction Scheme with
DOT Conventional Rebalance on Miller's
Problem Set

Problem	Iterations to Converge			
	DOT Conventional Rebalance	Source Correction Scheme		
		Miller's Results	Extrapolation Method	Boundary Ratio Method
M1	11	5	6	7
M2	26	5	6	8
M3	11	5	6	7
M4	26	5	6	8
M5	7	4	5	5
M6	6	4	5	5
M7	5	4	4	5

In any discrete ordinates calculation one would expect to achieve slower convergence for a problem in which the mesh width Δx is doubled when all other parameters remain the same. However, comparison of problems M3 and M4 shows that a doubling of Δx does not slow convergence in the SCS as much as it slows convergence in the DOT conventional rebalance method.

The mesh width, Δx , can also be expressed in terms of the mean free path, λ_t . The mean free path is the average distance a particle travels in a homogeneous medium before changing its direction or energy.¹ It is related to the total cross section as

$$\lambda_t = 1/\sigma \quad .^1 \quad (99)$$

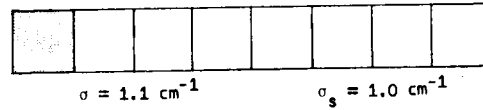
So for example in problems M1 and M3 the mean free path, $\lambda_t = 1$ cm and so $\Delta x = 1$ m.f.p. In problem M2 $\Delta x = 2$ m.f.p. Thus one would expect problem M2 to converge more slowly than problem M1. However the slowdown in convergence is more pronounced in the DOT CRB method than in the SCS.

The two methods of handling the void boundary conditions were compared on two other problems. These two methods are the boundary ratio method and the extrapolation method as described in Sect. IV.E.

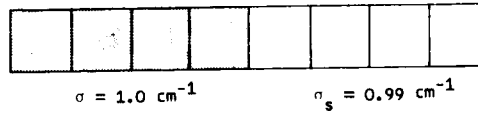
The two problems that were used to compare the boundary ratio method with the extrapolation method are described in Fig. 4. Both problems consist of a slab made up of one material which is 2 cm thick. It is divided into eight intervals of length .25 cm each. Both problems are P_0 calculations done with diamond differencing. They both had void boundaries. The total cross section, σ , and the scattering cross section, σ_s , are in Fig. 4.

The number of iterations required for convergence for the SCS with the extrapolation and boundary ratio methods are recorded in Table 4.

It is seen that the extrapolation method does not converge for a problem that has the extraneous source concentrated near the boundary. The reason for this is related to the fact that the extrapolation method



Problem 8



Problem 9

Fig. 4. Description of Problems 8 and 9. The extraneous fixed source is distributed in the shaded region.

Table 4

Comparison of the Boundary Ratio Method
with the Extrapolation Method

Problem	Iterations to Converge	
	Boundary Ratio	Extrapolation
8	11	*
9	5	*

*Did not converge.

used Eq. (74) to find the boundary fluxes. If the source is concentrated near the left boundary then $\phi_{0 \ 3/2}$ (the scalar flux at the right boundary of the left-most boundary cell) is large. Consequently $\phi_{0 \ 1/2}$ is calculated to be large. However, in reality $\phi_{0 \ 1/2}$ decreases rapidly at a void boundary. Thus the extrapolation method for a void boundary fails to converge when the fixed source is concentrated near the boundary.

For this reason the boundary ratio method is recommended.

This concludes the subsection on the one-dimensional slab geometry results.

B. Results in Two-Dimensional Slab Geometry

Four different versions of the source correction scheme as well as the DOT conventional rebalance were tested in two dimensions. The four methods of the SCS arise because there are two methods of performing step (iii) of the rebalance procedure (the Alcouffe or the modified flow term) and there are two methods of performing step (iv) of the rebalance procedure (the all moments or the scalar moment).

Table 5 has a description of the five different rebalance methods. Method I is the DOT conventional rebalance method. Methods II-V are different versions of the SCS. Method II is the method used by Alcouffe in his work at Los Alamos.³ Several problems were run so that these methods could be compared.

Table 5
The Five Methods of Rebalance for
Two-Dimensional Slab Geometry

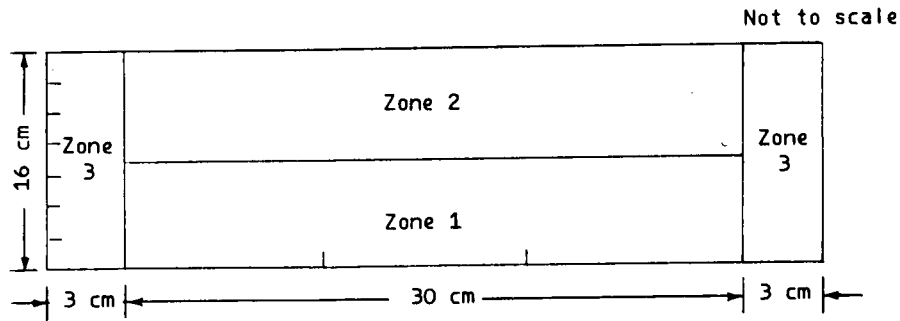
Method Number	Description of the Method	
	Method of Performing Step (iii) of the Rebalance Procedure	Method of Performing Step (iv) of the Rebalance Procedure
I	Conventional rebalance	All moments
II	Alcouffe's flow term (SCS)	Scalar moment
III	Alcouffe's flow term (SCS)	All moments
IV	Modified flow term (SCS)	All moments
V	Modified flow term (SCS)	Scalar moment

First a comparison is made between the four different versions of the SCS. All the SCS solutions were performed using the DOT-IV code along with the subroutine TWODIM. The four different versions can be grouped into two categories. Those methods which use the Alcouffe flow term (Methods II and III) are in one category. Those methods which use the modified flow term (Methods IV and V) are in another category. Methods III and IV were chosen as representatives from each category and were compared on several problems.

The problems have void boundaries and were solved using P-3 scattering expansion and S-8 directional quadrature. The super-weighted difference strategy was used in the solution of the transport equation [step (ii) of the rebalance procedure]. Four similar problems are described in Fig. 5a. Two other similar problems are described in Fig. 5b.

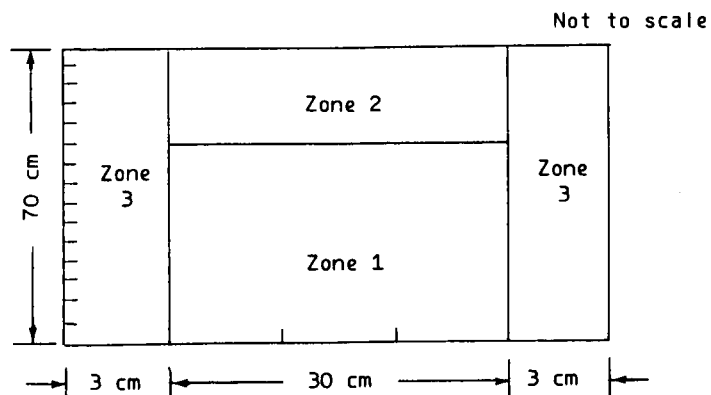
Alcouffe found that the SCS with his flow term was incompatible when used in conjunction with any difference strategy other than diamond differencing in the transport equation.³ From the derivation of the modified flow SCS it is evident that Method III is equivalent to Method IV when diamond differencing is used in the transport equation. However, as Table 6 shows, the SCS with the modified flow term is superior to the SCS with the Alcouffe flow term when a differencing strategy other than diamond differencing is used. Methods IV and V are the only methods that use the modified flow term.

The next question investigated is whether Method IV is superior to Method V. These two methods are compared in Table 7. It is seen that



Problem	Material in Zone		
	1	2	3
HC	Concrete	Concrete	Concrete
HS	Steel	Steel	Steel
HN	Sodium	Sodium	Sodium
H16	Sodium	Steel	Concrete

Fig. 5a. Problems HC, HS, HN, and H16.



Problem	Material in Zone		
	1	2	3
HRS	Sodium	Concrete	Concrete
H15	Sodium	Steel	Concrete

Fig. 5b. Problems HRS and H15.

Fig. 5. Description of Several Problems. An isotropic fixed source was distributed along the bottom row of mesh cells. Mesh boundaries are indicated at left and bottom.

Table 6
Comparison of Method III with Method IV

Problem	Iterations to Converge	
	Method III	Method IV
HC	16	9
HS	20	10
HN	10	6
H16	15	10
HRS	18	9

Table 7
Comparison of Method IV with Method V

Problem	Iterations to Converge	
	Method IV	Method V
HC	9	9
HS	10	10
HN	6	6
HRS	9	10
H15	12	13

Method IV converges slightly faster than Method V in two of the problems. Thus it is concluded that the best SCS method of those considered is Method IV which is the SCS with the modified flow term and the all moments method.

The next comparison to be made is one between the best SCS (Method IV) and the DOT conventional rebalance (Method I). This comparison is made on a large realistic test problem called HL. The description of HL is in Fig. 6. This problem simulates part of a reactor shield. It has void boundaries and was solved using P-3 scattering expansion and S-8 directional quadrature. The super-weighted difference strategy was used in the solution of the transport equation. This problem consists of fourteen energy groups. A comparison between the best SCS (Method IV) and the DOT conventional rebalance (Method I) for one outer iteration for problem HL is shown in Table 8.

Method IV shows a clear superiority over Method I.

Finally a comparison is made between all five methods on the first five energy groups of problem HL. The results of this comparison are in Table 9. Once more the superiority of the modified flow term - all moments SCS (Method IV) is seen.

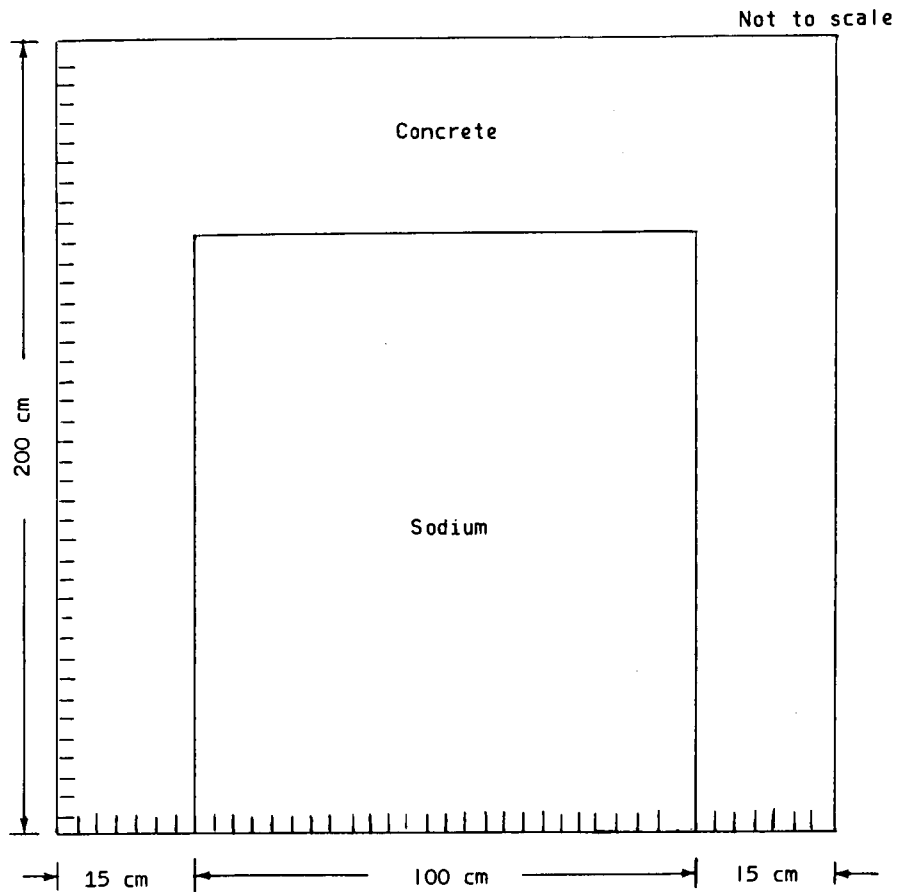


Fig. 6. HL — A Large Realistic Test Problem. An isotropic fixed source was distributed along the bottom row of mesh cells in the sodium region. Mesh boundaries are indicated at left and bottom.

Table 8
Comparison of Method I with Method IV
on Problem HL

Method	Iterations to Converge for Group													
	1	2	3	4	5	6	7	8	9	10	11	12	13	14
I	15	8	8	8	9	12	20	10	12	12	11	10	9	24
IV	12	8	7	7	8	8	9	8	8	8	8	8	8	10

Table 9
The First Five Groups of HL Run with
Each of the Five Methods

Method	Iterations to Converge for Group				
	1	2	3	4	5
I	15	8	8	8	9
II	15*	15*	15*	15*	15*
III	15*	15*	15*	15*	15*
IV	12	8	7	7	8
V	15*	15*	15*	15*	15*

*Did not converge in that many iterations.

VI. CONCLUSIONS

Finally the conclusions of this work are summarized. The SCS converges in fewer iterations than DOT conventional rebalance in both one and two dimensions.

In one-dimensional slab geometry the SCS is not slowed as much as the DOT CRB when a coarse mesh is used. Also problems with higher dominance ratio converge faster with the SCS than DOT CRB. Two methods of doing problems with void boundary conditions were compared in one-dimensional geometry — the extrapolation method and the boundary ratio method. The extrapolation method did not converge for problems that had a source concentrated near a boundary.

In two dimensions several SCS methods were compared. The best method was found to be Method IV which uses the modified flow term in the correction equation and the all moments method for finding the improved directional flux.

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VITA

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