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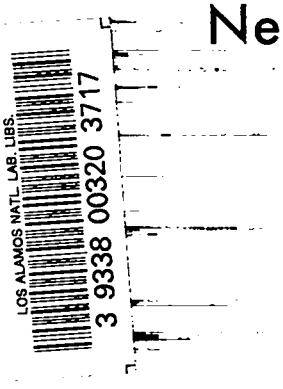

by

R. E. Alcouffe

*Work supported by the Division of Reactor Development and Technology, U. S. Atomic Energy Commission.

A GENERALIZED, FINITE-DIFFERENCED, DIFFUSION EQUATION FOR NEUTRON-TRANSPORT COMPUTATIONS

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ABSTRACT

A generalization of the neutron diffusion equation is derived which improves the results obtainable by conventional diffusion theory for multidimensional systems. The technique employs one-dimensional trial solutions to reduce the two-dimensional transport equation to the form of the neutron diffusion equation, thereby allowing the leakage terms to more closely approximate those appropriate for transport theory. A brief theoretical analysis shows that the accuracy of the generalized diffusion solution is linearly proportional to the difference between the trial solutions used and the exact transport solution. Four examples demonstrate the utility of the method for realistic systems for which a two-dimensional transport theory analysis is required. These results indicate that, even with an unsophisticated use of the trial solutions, the errors in integrated parameters are reduced to the order of a percent or less with the same computation time for the conventional diffusion calculation plus that required for the trial solution generation. It is also demonstrated that an accurate one-dimensional trial solution for every region of the system leads to a generalized diffusion equation that almost reproduces the transport theory results, consistent with the conclusions of the theoretical analysis.

I. INTRODUCTION

The neutronic characteristics of a nuclear reactor system are mathematically described by the linear Boltzmann transport equation. In this work, the reference numerical approximation to this equation is characterized as a multigroup, spatially finite-differenced equation with the angular variable approximated by using the discrete S_n method.[1,2] It can be shown that this numerical equation approximates the continuous equation to order $\sum_{i=1}^{N} \Delta\xi_i^2$ where $\Delta\xi_i$ is the mesh interval for the independent variable ξ_i. However, for multidimensional systems the solution to the numerical transport equation is relatively time consuming so that the computation is too expensive to perform routinely. An alternative description of the neutronics of a reactor system can be derived by assuming that the neutron transport is a diffusion process. The resulting neutron diffusion equation is in fact an approximation to the Boltzmann equation; its derivation therefrom is given in the Appendix. In general, the diffusion equation yields an accurate approximation to the transport solution if all of the following conditions are satisfied:

(1) the region of interest is far (greater than ~2 mfp) from any strong absorbers or any extraneous source,
(2) vacuum boundaries are far (> 2 mfp) from the region of interest,
(3) the transport cross section is used to define the diffusion coefficient and extrapolation length in regions of nonisotropic scatter, and
(4) $\Sigma a/\Sigma s \ll 1$ for the entire system.

These restrictions apply when the diffusion coefficient is defined in the conventional manner.

However, as is shown in the Appendix, one can derive the diffusion equation so that its solution exactly reproduces the angle-integrated flux of the transport equation. Unfortunately, one must know the transport flux and current in order to derive the exact diffusion coefficient. An intermediate approximation to the multidimensional transport equation, analogous to the exact procedure above but using approximate transport solutions of the system of interest, is derived in this work.

The motivation for basing a numerical transport approximation upon the diffusion equation is that considerable experience has been gained in obtaining efficient methods for computing solutions to the numerical diffusion equation. Also, because diffusion theory has been extensively used in nuclear reactor analysis, highly optimized computer codes to solve the multidimensional diffusion equation exist at almost all installations. The "generalized" diffusion equation, which is the result of using transport trial solutions of the system, retains all of the properties of the conventional form in that the matrix of the coefficients is symmetric and diagonally dominant. Therefore, to use this approximate method one need only alter the diffusion theory code to compute improved diffusion coefficients from given, but approximate, transport solutions while leaving the code logic and iteration schemes the same. These results are developed explicitly in the next section.

II. DERIVATION AND PROPERTIES OF THE GENERALIZED DIFFUSION EQUATION

In this section the generalized one-dimensional and two-dimensional numerical diffusion equation is derived to illustrate the important features and consequences of the method. Basically, the derivation procedes from the numerical form of the transport equation using the discrete S_n approach to account for the angle variables. Suitable trial functions for the flux are constructed which lead to reduced equations of the form of the numerical diffusion equation. To account for the transport effects not normally treated in diffusion theory, an S_n trial solution of the system is used in the trial function. From this generalized numerical diffusion equation, certain properties of its solution can be deduced based on the nature of the trial solutions used.

To demonstrate this the one-dimensional, one-group, S_n equation is written as

$$B\left[\phi_{i+\frac{1}{2},m},\phi_{im}\right] \equiv w_m\mu_m\left(A_{i+\frac{1}{2}}\phi_{i+\frac{1}{2},m} - A_{i-\frac{1}{2}}\phi_{i-\frac{1}{2},m}\right) + \left(A_{i+\frac{1}{2}} - A_{i-\frac{1}{2}}\right)\left(\alpha_{m+\frac{1}{2}}\phi_{i,m+\frac{1}{2}} - \alpha_{m-\frac{1}{2}}\phi_{i,m-\frac{1}{2}}\right) + w_m V_i\sigma_{ti}\phi_{im} - w_m V_i\sum_{m'=1}^{MM} w_{m'}\sigma_{sim'\to m}\phi_{im'} - w_m V_i S_{im} = 0 \quad , \tag{1}$$

$m=1,\cdots, MM,\ i = 1,\cdots, I$.

A general boundary condition is $\phi_{I+\frac{1}{2},m} = q_m$ for m such that $\mu_m < 0$, and I designates the rightmost, or outer, boundary of the system. The quantities in Eq. (1) are taken directly from Ref. 2 where they are appropriately defined for the specific geometry involved. Reduced equations that yield the diffusion equation form may be deduced by assuming, for both the boundary flux $\phi_{i+\frac{1}{2},m}$ and the spatial mesh-averaged flux ϕ_{im}, trial functions of the form[3]

$$\phi_{i+\frac{1}{2},m} = \frac{\psi_{i+\frac{1}{2},m}\left(a_{i+1} - a_i\right)}{\psi_{oi+1} - \psi_{oi}} \quad , \tag{2}$$

$$\phi_{im} = \frac{\psi_{im}\, a_i}{\psi_{oi}} \quad , \tag{3}$$

for $m=1,\cdots, MM$, and $i = 1,\cdots, I$,

where $\psi_{oi} = \sum_{m=1}^{MM} w_m\psi_{im}$, and a_i is the unknown quantity.

The form of the boundary fluxes is chosen so as to obtain a leakage term compatible with that of the numerical diffusion equation. It is assumed that the boundary flux and mesh-averaged flux, ϕ_{im}, are independent and that definitions (2) and (3) can be made consistently.

When Eqs. (2) and (3) are substituted into Eq. (1) and the summation over m is performed, the following equation for a_i results.

$$B\left[a_i\right] = R_i\left(a_{i+1} - a_i\right) - L_i\left(a_i - a_{i-1}\right) + \sigma_{Ti}V_i a_i - \sigma_{soi}V_i a_i - V_i S_{oi} = 0 \tag{4}$$

for $i=1,\cdots, I$,

where

$$R_i = \frac{\sum_{m=1}^{MM} w_m \mu_m A_{i+\frac{1}{2}} \psi_{i+\frac{1}{2},m}}{\psi_{oi+1} - \psi_{oi}} , \qquad (5)$$

$$L_i = R_{i-1} , \qquad (6)$$

$$\sigma_{soi} = \sum_{m=1}^{MM} w_m \sum_{m'=1}^{MM} w_{m'} \sigma_{si,m' \to m} , \qquad (7)$$

The leakage coefficient, R_i, at the rightmost boundary is defined to allow boundary conditions for a_i which are compatible with existing diffusion-theory codes; the trial solution is also assumed to satisfy the S_n transport boundary condition. For example, the vacuum boundary condition at the outside boundary in diffusion theory is $a_{I+1} = 0$; therefore, ψ_{oI+1} in Eq. (5) must be set to zero for consistency, i.e., in order to compute the right-hand leakage obtained from the transport equation solution. For reflecting boundary conditions, $R_I = 0$ and therefore is consistent with the diffusion equation. The periodic boundary condition can be written $a_1 = a_{I+1}$ and $a_0 = a_I$. A boundary source is treated using an appropriate source term with zero-flux boundary conditions.

Equation (4) is an obvious extension of diffusion theory in that the diffusion coefficient resulting from Fick's law can be generalized so that Eq. (5) is obtained for the leakage coefficient. However, derivation of Eq. (4) from Eq. (1) has the advantage that one gains some insight about the behavior of the solution to Eq. (4). For example, if Eqs. (5) and (6) are taken as prescriptions for the leakage coefficient, then one need use only the isotropic component of the scattering matrix without any so-called "transport corrections." This is true even for the multigroup case, as can easily be shown. Further, one can also reduce the number of both spatial and energy-mesh intervals by using the trial solutions consistently to increase the efficiency of the final computation (see Eqs. (17) to (21)).

At this point, it is fruitful to explore some of the consequences of using the trial solution ψ to derive the generalized diffusion equation. Assume that the trial solution is represented as

$$\psi_{im} = \phi_{im} + \varepsilon_{im} , \qquad (8)$$

where ϕ_{im} is the exact solution of Eq. (1) and ε_{im} is an error function. The leakage coefficient of Eq. (5) may now be evaluated as

$$R_i = \frac{\sum_m w_m \mu_m A_{i+\frac{1}{2}} \psi_{i+\frac{1}{2},m}}{\sum_m w_m (\psi_{i+1,m} - \psi_{im})}$$

$$= \frac{\sum_m w_m \mu_m A_{i-\frac{1}{2}} \phi_{i-\frac{1}{2},m}}{\sum_m w_m (\phi_{i+1,m} - \phi_{im})} + \frac{\sum_m w_m \mu_m A_{i-\frac{1}{2}} \varepsilon_{i+\frac{1}{2},m}}{\sum_m w_m (\psi_{i+1,m} - \psi_{im})}$$

$$\times \left[\frac{\sum_m w_m (\varepsilon_{i+1,m} - \varepsilon_{im})}{\sum_m w_m \mu_m A_{i+\frac{1}{2}} \varepsilon_{i+\frac{1}{2},m}} \; \frac{\sum_m w_m \mu_m A_{i+\frac{1}{2}} \phi_{i+\frac{1}{2},m}}{\sum_m w_m (\phi_{i+1,m} - \phi_{im})} - 1 \right]$$

$$\equiv R_{oi} + R_{Ei} . \qquad (9)$$

If the solution to Eq. (4) found using the trial solution ψ_{im} is expressed as $a_i = a_{oi} + a_{Ei}$ where $a_{oi} = \sum_{m=1}^{MM} w_m \phi_{im}$, then the equation may be rewritten as

$$(R_{oi} + R_{Ei})(a_{oi+1} - a_{oi}) + R_i(a_{Ei+1} - a_{Ei})$$

$$- (L_{oi} + L_{Ei})(a_{oi} - a_{oi-1}) - L_i(a_{Ei} - a_{Ei-1})$$

$$+ \sigma_{Ti} V_i (a_{oi} + a_{Ei}) - \sigma_{soi} V_i (a_{oi} + a_{Ei}) - V_i S_{oi} = 0. \qquad (10)$$

From the definition of R_{oi} from Eq. (9), it is evident that

$$R_{oi}(a_{oi+1} - a_{oi}) - L_{oi}(a_{oi} - a_{oi-1}) + \sigma_{Ti} V_i a_{oi}$$

$$- \sigma_{soi} V_i a_{oi} - V_i S_{oi} = 0 . \qquad (11)$$

Equation (11) is a statement that when the exact solution is used as the trial solution $(\psi_{im} = \phi_{im})$, then

$$a_i = \sum_m w_m \phi_{im}$$

is a solution of Eq. (4). Therefore, the equation for the error function from Eq. (10) becomes

$$R_i(a_{Ei+1} - a_{Ei}) - L_i(a_{Ei} - a_{Ei-1}) + \sigma_{Ti}V_i a_{Ei} - \sigma_{soi}V_i a_{Ei} = -\left[R_{Ei}(a_{oi+1} - a_{oi}) - L_{Ei}(a_{oi} - a_{oi-1})\right] . \quad (12)$$

Equation (12) has precisely the same form as Eq. (4) with a source term that reflects the difference between the exact solution to Eq. (1) and the trial solution used. The nature of this error source can be determined if we assume that the trial solution obeys the relationship

$$\frac{\sum_{m=1}^{MM} w_m \mu_m \psi_{i+\frac{1}{2},m}}{\sum_{m=1}^{MM} w_m (\psi_{i+1,m} - \psi_{im})} = -\frac{F_i D_i}{h_i} , \quad (13)$$

where h_i is the spatial mesh length, D_i is the conventional diffusion coefficient $(D_i = 1/3\ \Sigma_{tri})$, and F_i is a positive, finite function necessary to make the equality true. We may then write the source term as

$$S_{Ei} = \left[\frac{F_i D_i A_{i+\frac{1}{2}}}{h_i}(\epsilon_{oi+1} - \epsilon_{oi}) + A_{i+\frac{1}{2}}\epsilon_{1i+\frac{1}{2}} - \frac{F_{i-1}D_{i-1}A_{i-\frac{1}{2}}}{h_{i-1}}(\epsilon_{oi} - \epsilon_{oi-1}) - A_{i-\frac{1}{2}}\epsilon_{1i-\frac{1}{2}}\right],$$

where

$$\epsilon_{oi} = \sum_{m=1}^{MM} w_m \epsilon_{im} ,$$

$$\epsilon_{1i+\frac{1}{2}} = \sum_{m=1}^{MM} w_m \mu_m \epsilon_{i+\frac{1}{2},m} . \quad (14)$$

Equation (13) is crucial for determining the validity of the generalized diffusion method in that the function F_i is assumed to be positive and finite for the entire range of i. If this is true, then the matrix of the coefficients of Eqs. (4) and (12) is symmetric and diagonally dominant. This, in turn, guarantees a unique solution to both equations since this is the type of property possessed by the conventional numerical diffusion equation. At distances greater than ~2 mean free paths from material interface and sources, F_i should be a slowly varying function of the index i. The error source is proportional to ϵ_{oi} and ϵ_{1i}, and, if these quantities vanish, then the only solution to Eq. (12) is $a_{Ei} = 0$ for all i. Hence, if the trial solution is the exact solution of the system, the *unique* solution to Eq. (4) is

$$a_i = \sum_{m=1}^{MM} w_m \phi_{im} \text{ for all i.}$$

The source term can be rewritten if we assume that the exact transport solution ϕ_{im} also obeys Eq. (13) with a proportionally function G_i. Thus

$$S_{Ei} = \frac{G_i D_i A_{i+\frac{1}{2}}}{h_i}(\epsilon_{oi+1} - \epsilon_{oi}) - \frac{G_{i-1}D_{i-1}A_{i-\frac{1}{2}}}{h_{i-1}}(\epsilon_{oi} - \epsilon_{oi-1}) , \quad (15)$$

and, consequently, the source is proportional to the difference quantities, $\epsilon_{oi+1} - \epsilon_{oi}$. Because of the properties of the matrix of coefficient of Eq. (12), the inverse exists. This inverse is positive, and, therefore, the error quantity a_E is also proportional to ϵ_o. This property implies that, as the trial solutions approach the exact solution, the solution to the generalized diffusion equation likewise approaches the angle-averaged exact solution to the same order. This may be used to theoretically assess the usefulness of the trial solutions for certain classes of problems.

The extension of the generalized diffusion-equation approach from the one-dimensional derivation to two or three dimensions is straightforward. The development of the two-dimensional equation is presented here to demonstrate the use of the trial solutions to simultaneously collapse both the spatial and energy-mesh description of the two-dimensional system from that used to compute the trial solution. Also, one must consider the possibility of using several one-dimensional trial solutions of the system consistently to obtain an appropriate generalized diffusion equation.

The derivation follows from the two-dimensional, S_n transport equation written as follows.[2]

$$B\left[\phi^k_{i+\frac{1}{2},j,m}, \phi^k_{i,j+\frac{1}{2},m}, \phi^k_{ijm}\right] \equiv w_m\mu_m(A_{i+\frac{1}{2},j}\phi^k_{i+\frac{1}{2},j,m} - A_{i-\frac{1}{2},j}\phi^k_{i-\frac{1}{2},j,m}) + w_m\mu_m B_{ij}(\phi^k_{i,j+\frac{1}{2},m} - \phi^k_{i,j-\frac{1}{2},m}) + (A_{i+\frac{1}{2},j} - A_{i-\frac{1}{2},j})(\alpha_{m+\frac{1}{2}}\phi^k_{i,j,m+\frac{1}{2}} - \alpha_{m-\frac{1}{2}}\phi^k_{i,j,m-\frac{1}{2}})$$

$$+ \sigma^{k}_{Tij} w_m V_{ij} \phi^{k}_{kjm} - w_m \sum_{m'=1}^{MM} w_{m'} \sum_{k'=1}^{K} V_{ij} \sigma^{k' \to k}_{si,j,m' \to m} \phi^{k}_{ijm'}$$

$$- V_{ij} S^{k}_{ijm} = 0 \qquad (16)$$

for $m=1,\cdots,MM$, $i=1,\cdots,I$, $j=1,\cdots,J$, $k=1,\cdots,K$;

m is the angle index, i and j are spatial-mesh indices, and k is the energy-group index.

The trial functions are to be designed (1) to obtain the numerical-diffusion-equation form from the transport equation, (2) to allow the collapse of both the spatial mesh and the energy mesh used to compute the trial solutions to some coarse-mesh description, and (3) to utilize a two-dimensional trial solution. The practicality of the last point, using a trial solution with the same number of spatial dimensions as the problem to be solved, arises from the computation of perturbations of the system from some reference configuration. Examples are time-dependent analyses and survey type problems in which a specified design objective is to be attained by selected perturbations of the system.[4-6] The following trial functions for the boundary fluxes and mesh-averaged flux incorporate the above criteria.

$$\phi_{i_{\mu+\frac{1}{2}},j,m} = \frac{\psi^{k}_{i_{\mu+\frac{1}{2}},j,m} \left(a^{g}_{\mu+1,\nu} - a^{g}_{\mu\nu}\right)}{\psi^{g}_{\mu+1,\nu} - \psi^{g}_{\mu\nu}} \qquad (17)$$

for $j \epsilon \nu$, $k \epsilon g$, $m=1,\cdots,MM$;

$$\phi^{k}_{i,j_{\nu}+\frac{1}{2},m} = \frac{\psi^{k}_{i,j_{\nu}+\frac{1}{2},m} \left(a^{g}_{\mu,\nu+1} - a^{g}_{\mu\nu}\right)}{\psi^{g}_{\mu,\nu+1} - \psi^{g}_{\mu\nu}} \qquad (18)$$

for $i \epsilon \mu$, $k \epsilon g$, $m=1,\cdots,MM$;

$$\phi^{k}_{ijm} = \frac{\psi^{k}_{ijm}\, a^{g}_{\mu\nu}}{\psi^{g}_{\mu\nu}} \qquad (19)$$

for $i \epsilon \mu$, $j \epsilon \nu$, $k \epsilon g$, $m=1,\cdots,MM$;

where μ and ν indicate a coarse-mesh description in the i and j directions, respectively; each coarse-mesh interval contains an integral number of fine mesh intervals; and g is a broad-group description. Typical fine- and broad-mesh arrangements in one spatial direction are shown in Fig. 1A. Note that the boundary-flux expressions are defined for the coarse-mesh boundaries only; otherwise Eq. (19) is used. The average trial-solution flux used in Eqs. (17) to (19) is defined as

$$\psi^{g}_{\mu\nu} = \sum_{m=1}^{MM} \sum_{k \epsilon g} \sum_{i \epsilon \mu} \sum_{j \epsilon \nu} w_m V_{ij} \psi^{k}_{ijm} \Big/ V_{\mu\nu} \,. \qquad (20)$$

If trial functions (17) to (19) are substituted for the relevant quantities in Eq. (16) and the indicated summations are carried out, the following two-dimensional numerical-diffusion equation results.

$$B\left[a^{g}_{\mu\nu}\right] = R^{g}_{\mu\nu}\left(a^{g}_{\mu+1,\nu} - a^{g}_{\mu\nu}\right) - L^{g}_{\mu\nu}\left(a^{g}_{\mu\nu} - a^{g}_{\mu,\nu-1}\right)$$
$$+ T^{g}_{\mu\nu}\left(a^{g}_{\mu,\nu+1} - a^{g}_{\mu\nu}\right) - B^{g}_{\mu\nu}\left(a^{g}_{\mu\nu} - a^{g}_{\mu,\nu-1}\right)$$
$$+ \Sigma^{g}_{T\mu\nu} V_{\mu\nu} a^{g}_{\mu\nu} - \sum_{g'=1}^{G} V_{\mu\nu} \sigma^{g' \to g}_{so\mu\nu} a^{g'}_{\mu\nu} - V_{\mu\nu} S^{g}_{\mu\nu} = 0, \qquad (21)$$

where

$$R^{g}_{\mu\nu} = \frac{\sum_{m=k}^{MM} \sum_{k \epsilon g} \sum_{j \epsilon \nu} w_m \mu_m A_{i_{\mu+1}+\frac{1}{2},j} \psi^{k}_{i_{\mu+1}+\frac{1}{2},j,m}}{\psi^{g}_{\mu+1,\nu} - \psi^{g}_{\mu,\nu}} \,,$$

$$L^{g}_{\mu\nu} = R^{g}_{\mu-1,\nu} \,,$$

$$T^{g}_{\mu\nu} = \frac{\sum_{m=1}^{MM} \sum_{k \epsilon g} \sum_{i \epsilon \mu} w_m \mu_m B_{i,j_{\nu+1}} \psi^{k}_{i,j_{\nu+1}+\frac{1}{2},m}}{\psi^{g}_{\mu\nu+1} - \psi^{g}_{\mu\nu}} \,,$$

$$B^{g}_{\mu\nu} = T^{g}_{\mu,\nu-1} \,,$$

$$V_{\mu\nu}\, \Sigma^{g}_{T\mu\nu} = \frac{\sum_{m=1}^{MM} \sum_{k \epsilon g} \sum_{i \epsilon \mu} \sum_{j \epsilon \nu} w_m V_{ij} \sigma^{k}_{Tij} \psi^{k}_{ijm}}{\psi^{g}_{\mu\nu}} \,,$$

$$V_{\mu\nu}\, \sigma^{g' \to g}_{so\mu\nu} = \frac{\sum_{k \epsilon g} \sum_{k' \epsilon g'} \sum_{i \epsilon \mu} \sum_{j \epsilon \nu} V_{ij} \sigma^{k' \to k}_{soij} \psi^{k'}_{oij}}{\psi^{g'}_{\mu\nu}} \,,$$

$$V_{\mu\nu}\, S^{g}_{\mu\nu} = \sum_{m=1}^{MM} \sum_{k \epsilon g} \sum_{i \epsilon \mu} \sum_{j \epsilon \nu} w_m V_{ij} S^{k}_{ijm} \,. \qquad (22)$$

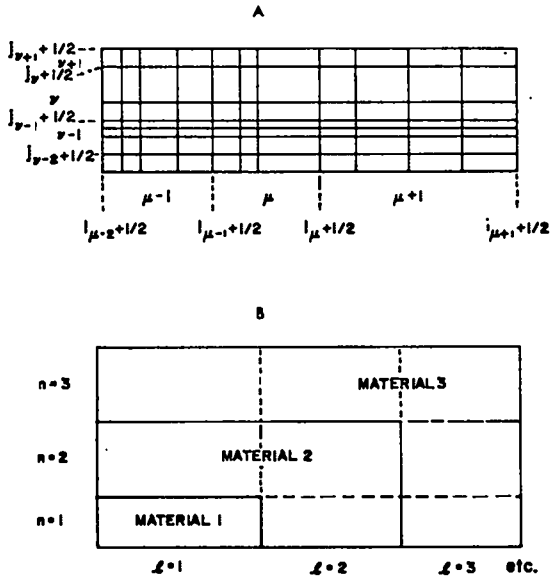

Fig. 1. Some geometrical considerations useful to the generalized diffusion equation method.

Equation (21) has the same property as that outlined for the one-dimensional, generalized diffusion equation; if the exact solution of the system is used as the trial solution, the generalized equation yields the solution

$$a^g_{\mu\nu} = \phi^g_{\mu\nu},$$

regardless of how the mesh intervals in space or energy are partitioned. This result is very important in that for a series of calculations on variations of the system, the fine-mesh, fine-group computation need be performed only once. The broad-mesh description can then be chosen to concentrate upon the area where the perturbation most affects the flux in order to obtain an accurate calculation of the perturbation of the system. The same type of result carries over when one-dimensional trial solutions are used to compute two-dimensional systems.

The generalized diffusion equation method is more useful if one-dimensional trial solutions of the two-dimensional system of interest are used to derive the two-dimensional equation whose solution gives an accurate estimate of the true two-dimensional equation transport flux. The prescription for computing such trial solutions is not fixed, but, basically, the aim is to obtain one-dimensional estimates of the leakage in each spatial direction through the regions of the system where transport effects are assumed to be important. If such trial solutions are available, the following procedure for defining the trial functions is used.

(1) Assume that the trial solutions are generated from a series of runs through relevant regions of the system in each of the transverse directions (the R and Z directions).* These can be ordered as ψ^n_{Rim}, n=1,···, K, implying a sequence of radial calculations for each axial elevation n. Similarly, the axial trial solutions are ψ^ℓ_{Zjn}, ℓ=1,···, L for each radial interval ℓ.

(2) Define the trial functions as

$$\phi_{i+\frac{1}{2},j,m} = \frac{\psi_{Ri+\frac{1}{2},m}\left(a_{i+1,j} - a_{ij}\right)}{\psi_{Roi+1} - \psi_{Roi}} \qquad (23)$$

for jεn, n=1,···,k ;

$$\phi_{i,j+\frac{1}{2},m} = \frac{\psi^\ell_{Zj+\frac{1}{2},m}\left(a_{i,j+1} - a_{ij}\right)}{\psi_{Zoj+1} - \psi_{Zoj}} \qquad (24)$$

for iεℓ, ℓ=1,···,L ; and

$$\phi_{ijm} = a_{ij} \text{ for all i and j.} \qquad (25)$$

These trial functions can be further generalized to include the possibility of both space and energy collapse in the manner used in Eqs. (17) to (19).

If the above strategy is pursued, the problem is in obtaining one-dimensional trial solutions that accurately represent the two-dimensional flux through each of the regions at each elevation. This problem is solvable with existing one-dimensional S_n codes if for each traverse through the system of interest: (1) a predominant source is available, (2) an asymptotic transport solution** is obtained in each region including the transverse-leakage behaviour, and (3) a simple buckling approach is sufficient to account for the transverse leakage. Condition (1) can be relaxed if the region of interest can be adequately described by diffusion theory. This gives rise to some important applications of the method, one of which is given by Example 3 in Section III. Condition (3) also can be relaxed if

*See Fig. 1B.

**An asymptotic transport solution is one in which the ratios $j_x(x,y)\,\frac{\partial\phi}{\partial x}$ and $j_y(x,y)\,\frac{\partial\phi}{\partial y}$ become constant in a region.

some consistent scheme for estimating the transverse leakage by introducing a source from a previous two-dimensional computation is possible. This is further discussed in Section IV.

Three-dimensional problems can be similarly solved by an analogous choice of trial functions and and trial solutions. Although the method can be formulated using two-dimensional trial solutions, it would be much more economical to use one-dimensional trial solutions in each of the three space directions. If this is done, the logic used for computing trial solutions does not change from the two-dimensional case, which facilitates conversion from a two-dimensional to a three-dimensional analysis.

III. SELECTED NUMERICAL RESULTS

A variety of systems that exhibit two-dimensional transport effects have been computed to assess the applicability of the generalized diffusion method that uses one-dimensional transport trial solutions to compute the two-dimensional systems. When an exact two-dimensional transport solution is given, it has been computed using the TWØTRAN code. All time comparisons using the CDC 6600 are iteration times unless otherwise noted. The generalized diffusion results were obtained with an experimental code TWØDS which computes the trial solutions, performs the necessary calculations to compute the space- and energy-collapsed leakage coefficients, and then executes the two-dimensional diffusion calculation. The time required for solution by the generalized approach includes the computation time for the trial solutions and the leakage coefficients.

Example 1.

The first example is a small, fast system with a core of 95% Pu-239 and 5% Pu-240 fully reflected by natural uranium. The geometry is cylindrical with a core radius of 3 in. and a height of 1.55 in. The reflector is 3 in. thick. The analysis was done with nine energy groups (consisting of the first nine Hansen-Roach groups); the spatial mesh for a quadrant of the system is 15 by 15 mesh intervals, 5 by 5 of them in the core region. Table I is a summary of relevant computations, and Fig. 2 is a schematic of the system. The reference is a TWØTRAN S-12 computation of the system, and all numbers quoted are percent deviations from those results.

In this particular system, the average mean free path is 1.5 in. (3.9 cm); therefore it is neutronically small, and the main transport effect is leakage. Also, for this system ray effects seem to be important for the computation of detailed leakage rates; therefore, a high-order S_n computation is necessary for the reference. The GDE_0 column in Table I is a generalized diffusion calculation using one set of trial solutions through the core region radially and axially. In these one-dimensional calculations, a single buckling correction was used to account for the transverse leakage. Reflector region 4 was treated with the diffusion approximation, as were region 2 in the axial direction and region 3 in the radial direction. This is illustrated in Fig. 2 where the abbreviation GD indicates leakages computed from trial solutions and

TABLE I

EVALUATION OF EXAMPLE 1 USING THE GENERALIZED DIFFUSION EQUATION APPROACH

		Percent of Deviation From S-12				
	S-12	S-6	S-4	GDE_0	GDE_1	DE
k_{eff}	1.0423	0.29	0.78	0.07	0.35	-15.4
Core absorptions	0.29562	0.46	1.23	-0.71	—	-21.62
Reflector absorptions	0.17922	-0.29	-0.69	3.52	—	8.81
Radial leakage	0.25587	-0.43	1.15	-3.19	-0.30	8.06
Axial leakage	0.26930	0.10	-1.99	1.56	-0.04	10.25
Total leakage	0.52517	-0.16	-0.46	-0.76	-0.18	9.16
Iteration time (sec)	405[a]	173[a]	210	28.7	—	11

[a] A flux guess provided from the lower order calculation.

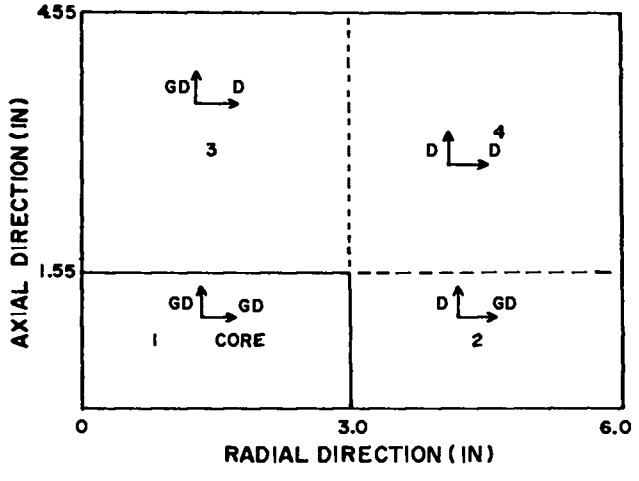

Fig. 2. Schematic representation of the systems for Examples 1 through 3.

D is the conventional diffusion leakage term. As can be seen, the two-dimensional generalized diffusion calculation gives about the same accuracy as the S-6 computation in the core region but is worse than the S-4 computation in the reflector region.

To determine the effect of good trial solutions through the core and the reflector, the two-dimensional S-12 fluxes were averaged over the core and reflector regions to give one-dimensional trial solutions for each region (one radial trial solution through regions 1 and 2, one through regions 3 and 4, and analogous functions in the axial directions). The results are presented in the column headed GDE_1 in Table I and show greatly improved accuracy, particularly in the reflector regions. That conventional diffusion theory does not apply in this case is shown by the result column headed DE.

Figure 3 shows the trial solutions used for the generalized diffusion equation and group 4, the dominant group. The S-12 trial solution is derived from the two-dimensional reference transport computation. We see that the trial solution computed from the one-dimensional pass with the transverse leakage accounted for by a simple buckling underestimates the flux in the reflector region. However, the generalized diffusion flux in the radial direction through the core derived using the above trial solution appears to be quite accurate. The chief error is in approximating the reflector region by the conventional diffusion coefficient. This is demonstrated in Fig. 4 which gives the radial fission density through the core (regions 1 and 2) and through the axial reflector (regions 3 and 4). The fission density computed using the generalized diffusion approach approximates the S-12 results very well through the core. However, in the axial reflector the results are high. The TWØTRAN S-4 results are also included as a point of reference for the errors incurred for few-angle S_n and to demonstrate the presence of ray effects in the reflector. The generalized diffusion solution with trial solutions from the S-12 TWØTRAN computation is much better than the results presented in Fig. 3, particularly in the reflector regions. Therefore, if one could devise a method to generate improved trial solutions in the nonsource reflector regions, the generalized diffusion solution would probably show a corresponding improvement. At present, no method for generating nonsource-region trial solutions has been found satisfactory for multigroup problems.

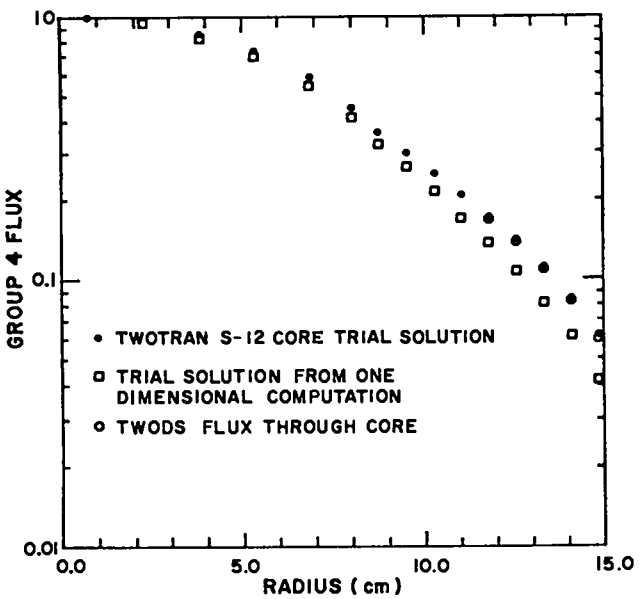

Fig. 3. Trial solution plus exact and GDE solution through core region of Example 1.

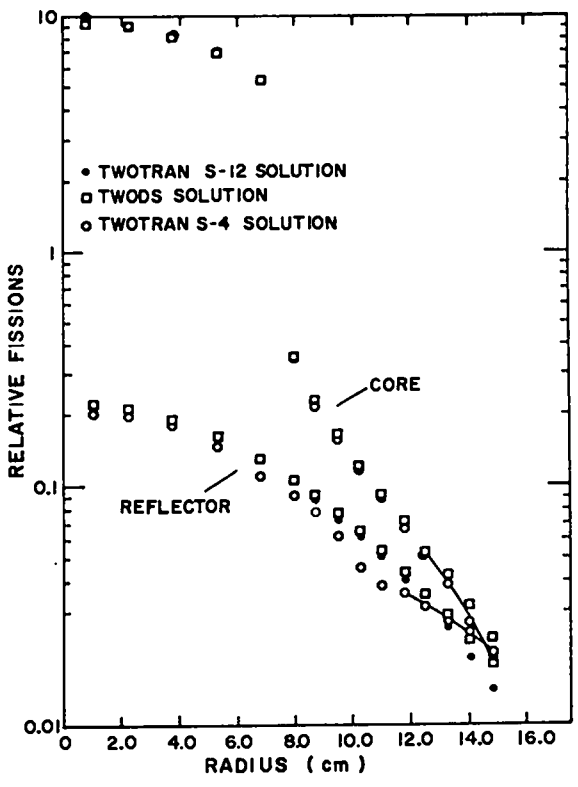

Fig. 4. Radial fission density through core and axial reflector of Example 1.

Example 2.

The second example is a core of fully enriched (93% U-235) uranium with a 4-in.^{2} cross section. The reflector is 9-in.-thick natural uranium. The same cross-section set was used as for Example 1. The spatial mesh for a quadrant of the system was 5 by 5 in the core and 15 by 15 total. The mean free path for the system is 1.3 in. for the core and 0.95 in. in the reflector; therefore, the core is neutronically small and the reflector is large. Again, because of the ray effect in the reflector region an S-12 calculation was necessary for the reference. Table II shows some calculational results for the system.

In the column headed S-4 are TWØTRAN S-4 results showing the magnitudes of errors incurred in that approximation. In the GDE column are generalized diffusion results obtained using trial solutions through the core region only, the transverse leakage being estimated using the simple buckling approach. The reflector, as in Example 1, is treated by the conventional diffusion approximation. In Fig. 5 the trial solution for group 3 is presented along with the averaged S-12 flux through the core. Table II column GDE_2 presents results of a generalized diffusion solution with trial solutions computed as described above except that group- and zone-dependent buckling was used. The appropriate bucklings were computed from the generalized diffusion solution of GDE_1. The results show an improvement in the core region, in particular, and slight improvement in the reflector. This trial solution is also shown in Fig. 5. The generalized diffusion fission density results are presented with S-12 and S-4 fission density results in Fig. 6. As in

TABLE II

EVALUATION OF EXAMPLE 2 USING THE GENERALIZED DIFFUSION EQUATION APPROACH

		Percent of Deviation From S-12			
	S-12	S-4	GDE_1	GDE_2	DE
k_{eff}	1.3913	0.39	0.69	0.07	-4.03
Core absorptions	0.5248	0.56	0.88	0.04	-5.75
Reflector absorptions	0.3927	-0.79	-0.05	-0.03	6.77
Leakage	0.08250	0.17	-5.21	-2.62	4.34
Core fissions	0.4884	0.59	0.69	0.50	-6.35
Reflector fissions	0.08416	0.77	0.73	0.61	9.48
Time (sec)		232	30.0	46.8	11.4

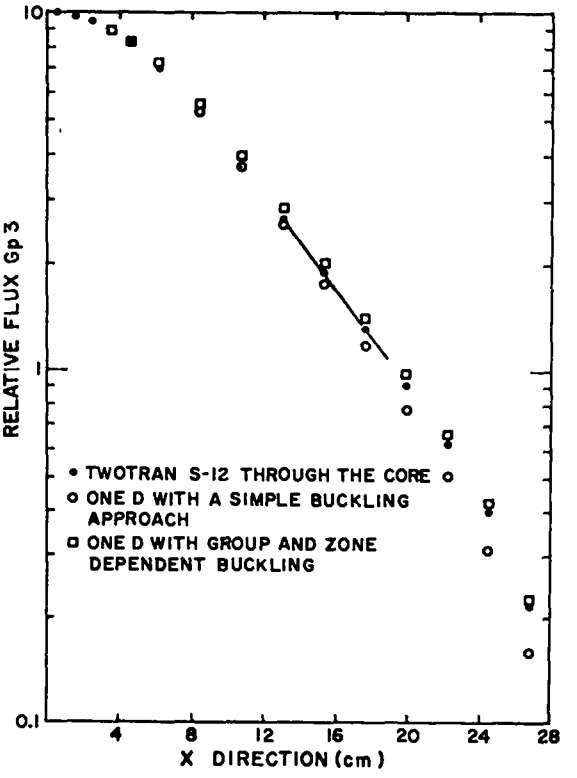

Fig. 5. Trial solutions plus exact solution through core region of Example 2.

Example 1, the results through the core are accurate but there are some deviations in the reflector. The chief source of leakage error is in the reflector region because of the diffusion approximation; therefore, a valid reflector trial solution should improve the results still more. The conventional diffusion solution results are presented in Table II column DE.

These two examples represent a severe test of the method because the multidimensional transport effects are large. That the simple use of core trial solutions only is so much better than a conventional diffusion theory calculation is remarkable. Example 1 also demonstrates that the accuracy can be further improved by using additional trial solutions which are an improvement over the diffusion approximation. This, therefore, suggests an interaction procedure whereby trial solutions are rederived from information supplied by the two-dimensional results to obtain more accurate results. One scheme for doing this is discussed in section IV and is alluded to in the improved results of Example 2 obtained by using group- and zone-dependent bucklings.

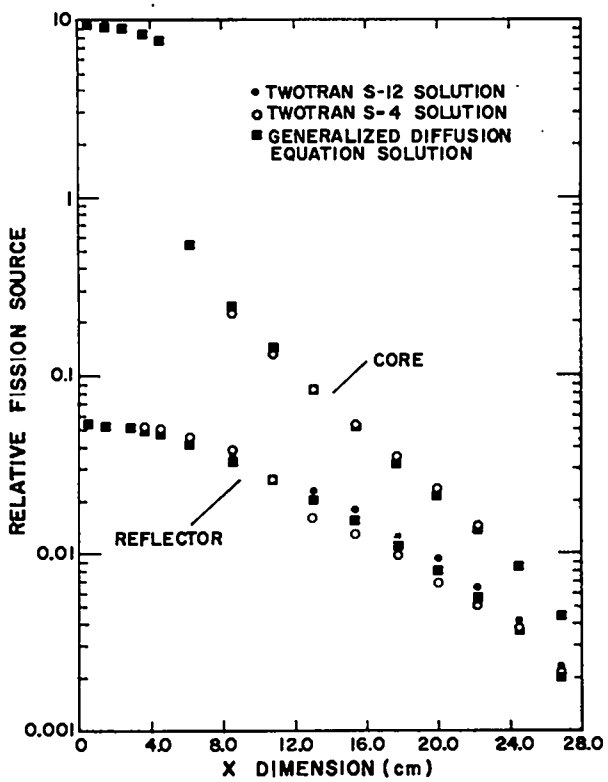

Fig. 6. X-Direction fission density through core and reflector region of Example 2.

Example 3.

The third example is a deep-penetration problem like that encountered in shielding applications. The system geometry can again be represented by Fig. 2 where the core contains a spatially flat source in a rectangular area bounded by the axes, x = 65 cm, and y = 60 cm. The entire model is 133 by 140 cm long, with an average mean free path of 20 cm. The system is homogeneous, with two-group cross sections given in Table III, and the boundary conditions are reflective on the bottom, left, and top boundaries and vacuum on the right. No TWØTRAN computation was done for the problem, but an essentially exact (P-19, 133 by 140 mesh) solution from which flux comparisons may be made has been computed for the fully reflective system. Also, because of the boundary conditions a one-dimensional computation through the source region and to the vacuum boundary yields a leakage that the two-dimensional computation must reproduce when the two-dimensional leakage is integrated over the length of the vacuum boundary. This is true for each group, assuming that the energy-integrated source is normalized to unity for each calculation.

TABLE III

PARAMETERS FOR COMPUTATION OF EXAMPLE 3

	Group 1	Group 2
Σ_a	0.061723	0.096027
$2\Sigma_f$	0.0	0.0
Σ_T	0.092104	0.100877
$\Sigma_s^{g\to g}$	0.006947	0.004850
$\Sigma_s^{g-1\to g}$	0.0	0.023434
Source density	0.006546	0.017701

A generalized diffusion computation of the system was made using one-dimensional, S-8 trial solutions through the source region in both the x and y directions. The trial solutions were computed with one mesh point per centimeter and were used to space collapse the description to 40 by 40 mesh intervals. The reflector was treated using the asymptotic transport value to determine the quantity

$$F_i = -\frac{\sum_{m=1}^{MM} w_m \mu_m \psi_{i+\frac{1}{2},m}}{\sum_{m=1}^{MM} w_m (\psi_{i+1,m} - \psi_{im})} \cdot \frac{h_i}{D_i} , \qquad (26)$$

where $D_i = \frac{1}{3\Sigma_{Tr}}$ is a constant taken from Table III. The trial solution used to evaluate Eq. (26) is either of those described above and is far from the source and vacuum boundary. It was found that F_i approached a constant value of 2.0 probably because of the large value of Σ_a/Σ_T. As evidenced from the large errors in conventional diffusion theory (Table IV), a value of $F_i = 1$ contributes to the inaccuracy of that solution.

Some calculational results are shown in Table IV and in Figs. 7 and 8. The ONED column of Table IV gives the one-dimensional S-8 results through the source and vacuum boundary (regions 1 and 2) with the results normalized to a total source of 1 neutron/cm^3/sec. The entries labeled Absorption 1 and Absorption 2 are the absorptions in the source and nonsource regions which the two-dimensional calculation should also reproduce if the absorption reaction rate is integrated over y for each region. In the GDE column are the generalized diffusion results obtained using the above described trial solutions, and in column DE are the conventional

TABLE IV

CALCULATIONAL RESULTS FOR EXAMPLE 3

		Percent of Deviation From ONED	
	ONED	GDE	DE
Leakage			
Group 1	5.517×10^{-6}	-1.69	-92.88
Group 2	8.814×10^{-6}	-0.44	-92.55
Absorption 1			
Group 1	0.1879	-0.02	-0.49
Group 2	0.7704	-0.03	-0.44
Absorption 2			
Group 1	0.008640	0.84	11.04
Group 2	0.03386	0.75	10.19
Time (sec)	1.9	13.9	7.2

diffusion results. The execution times are for the CDC 7600; the 6600 would require about a factor of four longer. The results presented in Figs. 7 and 8 are the group-1 fluxes as a function of x (through the vacuum boundary) for two y elevations, 1 mfp from the source and at the top reflecting boundary.

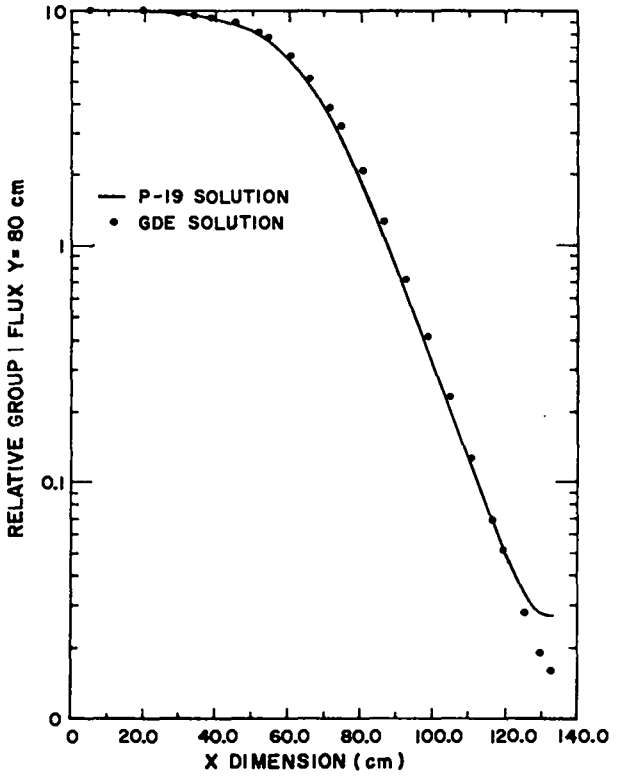

Fig. 7. Group-1 flux as a function of x at one mean free path from source region of Example 3.

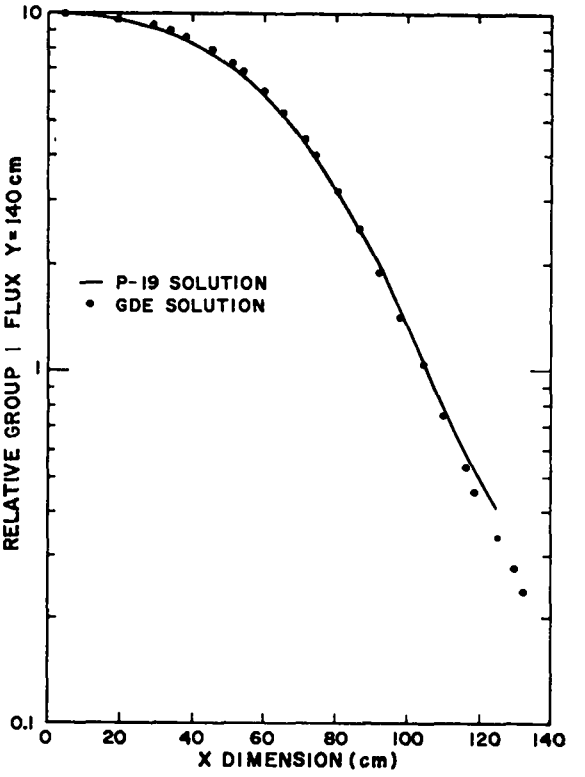

Fig. 8. Group-1 flux as a function of x at top boundary of Example 3.

The discrepancies around $x \geq 120$ cm are due to the use of a reflecting boundary for the reference computation. It should be noted that the conventional diffusion flux at the vacuum boundary is low by a factor of from 10 to 100. The good accuracy of the generalized diffusion approach in this particular example shows that the method is useful in deep-penetration or shielding-type problems that require more than one dimension for their analysis.

Example 4.

This example is presented to demonstrate the utility of the generalized diffusion equation in analyzing real reactor systems. The TREAT reactor is to be used by LASL for transient testing of mixed carbide and mixed nitride fuels to assess their usefulness for fast breeder reactor systems. To simulate a fast flux environment, the thermal flux from TREAT is to be shielded from the experimental pin by a gadolinium filter. The primary objectives of a neutronic analysis of the experiment are to determine (1) the radial and axial distributions of fissions in the pin and (2) the ratio of the power density in the experimental pin to the power produced in the reactor. Adequate representation of the

reactor and the experiment requires that the neutron thermalization be treated explicitly with neutron upscattering, and, because of the filter, the epithermal region must also be accounted for in detail. To this end 5 thermal and 17 epithermal (from 3 keV to 0.8 eV) groups, with a total of 29 groups for the entire energy range, were used. The anisotropic scatter of the graphite medium was also accounted for explicitly.

A TWØTRAN solution of this system was not attempted because the cost would be prohibitive owing to the large number of energy groups, the upscatter, and the many spatial mesh points. However, some indication of the accuracy of the solution computed using the two-dimensional generalized diffusion approach can be gained from the one-dimensional results and the two-dimensional conventional diffusion computation of the reactor. The generalized diffusion analysis was performed using a trial solution radially through the experimental pin and center of the reactor core. The reactor core and reflectors are adequately treated by diffusion theory so trial solutions through these regions are unnecessary. An axial trial solution through the pin region is desirable, but, because of the difficulty in obtaining a realistic formulation for a source in that region, such a computation is not yet possible.

The trial solution was used to collapse the radial spatial mesh from 89 to 41 mesh points, and the thermal groups from 5 to 1. That such a collapse gives accurate results is verified in Fig. 9 where the mesh-averaged, one-dimensional thermal flux is shown along with that obtained from the two-dimensional generalized diffusion computation at the midplane of the system.* The errors are well within

*In this particular case, the filter was not present, but its inclusion does not affect the general results.

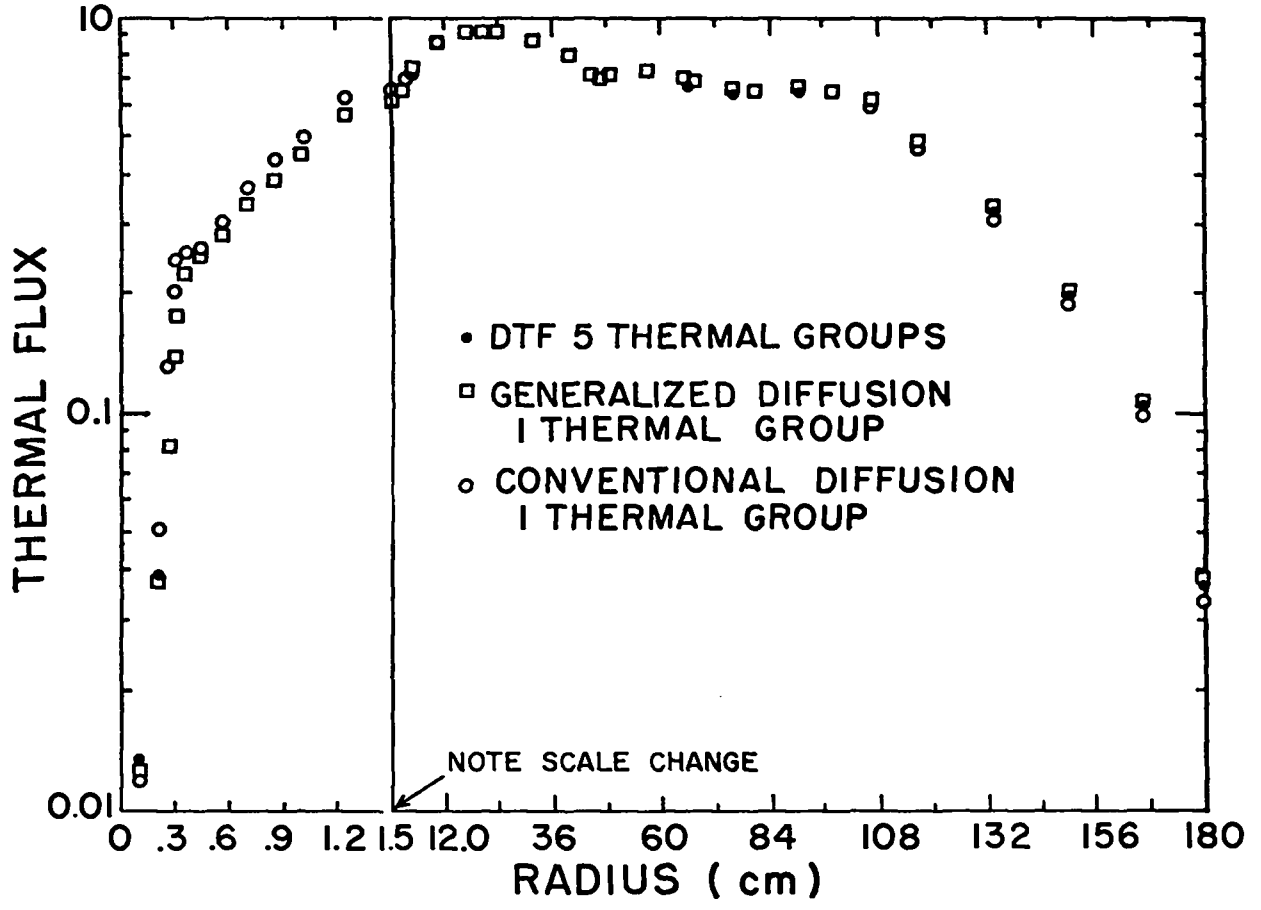

Fig. 9. Radial thermal neutron flux through core and experimental pin of Example 4.

±5%. Also shown for comparison are the results of a conventional two-dimensional diffusion computation. Figure 10 shows the radial distributions of fissions in the pin for the three computations. The difference between the one-dimensional and generalized diffusion results is due to an error in the spectrum at the center of the pin; this error is thought to be caused by a defect in the one-dimensional trial solution where for the high-energy groups the relationship of Eq. (13) does not hold because F_i changes sign in the central region of the pin due to numerical difficulties.

Some further results on the figure of merit (ratio of power density in the pin to the power in the reactor) and on system leakages and reaction rates are given in Table V.

It is felt that the generalized diffusion method has been a great help because the one-dimensional computations, which were necessary anyway for scoping, were used to obtain two-dimensional estimates of the quantities of interest for the system. The elimination of the need for two-dimensional upscattering calculations is especially beneficial in this case because they are inordinately time consuming. As is seen from the results of an equivalent conventional diffusion calculation, significant errors in the figure of merit have been eliminated and this would not have been possible otherwise.

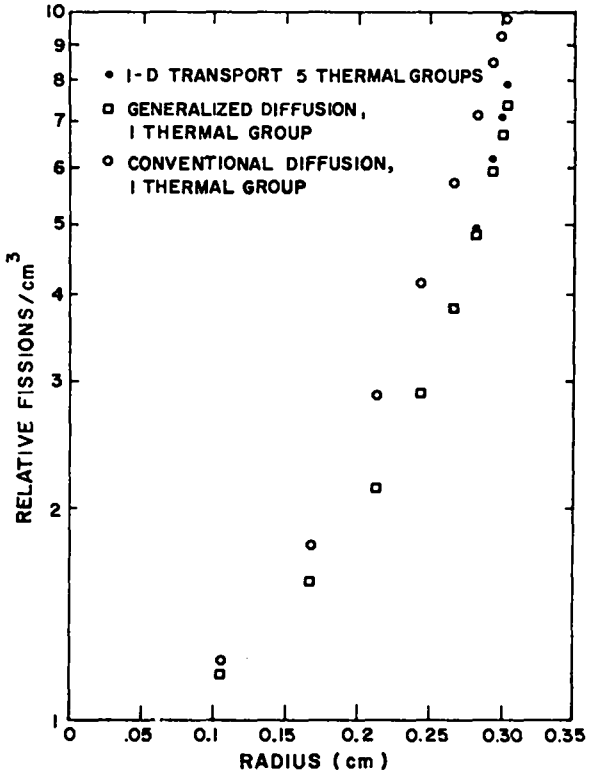

Fig. 10. Radial fission density through experimental pin of Example 4.

TABLE V

CALCULATIONAL RESULTS FROM EXAMPLE 4

	DTF-29 Group	Percent of Deviation from DTF-29 Group: GDE	DE
Total leakage	0.03558	-0.42	-1.85
Total fissions in experimental pin	0.004586	-2.37	33.48
Reactor	0.99541	0.01	-0.15
Figure of merit watt/cm³/reactor watts	--	1.024×10^{-4}	1.339×10^{-4}

IV. CONCLUSIONS AND RECOMMENDATIONS

Both the analysis and the realistic examples presented here show that the generalized diffusion equation method is a valuable approximation for multidimensional neutron-transport computations. It has been shown both analytically and empirically (Example 1) that if accurate trial solutions are available for the system of interest, the method will yield an accurate approximation to the two-dimensional, angle-averaged flux throughout the system. The following are important attributes and consequences of the method.

(1) The form and properties of the numerical generalized diffusion equation are the same as those of the diffusion equation; therefore, the iteration and acceleration techniques used to solve the latter are valid for the former.

(2) No extensive code development is necessary to solve the generalized diffusion equation. Modifications are needed only to provide for reading in the leakage coefficients and possibly for interfacing with codes that generate the trial solutions.

(3) The trial solutions are useful not only to account for strictly transport effects but also to reduce the spatial mesh and number of energy groups to a minimum, depending on the nature of the problem.

(4) One can develop theoretical analyses of the influence of the trial solutions upon the accuracy and validity of the solution of the generalized diffusion equation. It has been shown that the error in the solution is in some way proportional to the difference between the trial solution and the exact solution of the problem.

(5) The fact that the approximation method is based upon the diffusion equation ensures confidence that the solution is not unphysical or anomalous. This arises from the fact that a reasonable trial-solution calculational strategy can be automated and hence is not as user-dependent as the synthesis methods. Where accurate trial solutions cannot be computed, the conventional diffusion approximation is made, thereby ensuring a result at least as valid as diffusion theory.

(6) There is a significant time savings over the detailed two-dimensional transport solution, in the neighborhood of a factor of 10 for large problems. This also makes some three-dimensional analysis feasible.

These points demonstrate that the generalized diffusion-equation approach is theoretically very attractive and is useful for many practical reactor physics problems. When questions as to the accuracy of the solution to the equation arise, the crucial consideration is the ability of the one-dimensional trial solutions to represent the leakage (more exactly, the quantity F_i of Eq. (13)) for the two-dimensional system in each spatial direction and through each region. This suggests that the representation of two-dimensional systems by one-dimensional computations, particularly for nonsource regions, should be studied. In the examples presented, only trial solutions through source regions were computed because such a computation is straightforward with the S_n code available. Transverse-leakage effects were accounted for by a single buckling approximation (i.e., $\text{leakage}_i = -D_i^g B_i^2 = \Sigma_{Tri}^g X_i^{g2}$ where $X_i^g = \pi/[\sqrt{3}(\Sigma_{Tri}^g\, h + 1.42)]$, and h is the height). These trial solutions may be improved, and some estimate of the trial solutions for nonsource regions also may be obtained by generalizing the above approach. It is proposed that the information on the two-dimensional leakage developed in the generalized diffusion solution be used to recompute the trial solutions, thereby giving a presumably more accurate trial solution. To demonstrate the feasibility, consider the angle-integrated two-dimensional transport equation,

$$\frac{\partial j_x(x,y)}{\partial x} + \frac{j_y(x,y)}{\partial y} + \Sigma_T(x,y)\phi_o(x,y) - S_o(x,y) = 0. \tag{27}$$

Integrate this over a region along the y axis

$$\left[y_{j-\frac{1}{2}}, y_{j+\frac{1}{2}}\right] .$$

$$\frac{d\bar{j}_x(x)}{dx} + \frac{j_y(x,y_{j+\frac{1}{2}}) - j_y(x,y_{j-\frac{1}{2}})}{\Delta y_h} + \Sigma_{Tj}(x)\Phi_o(x) - \bar{S}_o(x) = 0 , \tag{28}$$

where

$$\Sigma_{Tj}(x) = \int_{y_{j-\frac{1}{2}}}^{y_{j+\frac{1}{2}}} \Sigma_T(x,y)\phi_o(x,y)dy/\Phi_o(x)\Delta y_j ,$$

$$\Phi_o(x) = \int_{y_{j-\frac{1}{2}}}^{y_{j+\frac{1}{2}}} \phi_o(x,y)dy/\Delta y_j ,$$

$$\bar{j}_x(x) = \int_{y_{j-\frac{1}{2}}}^{y_{j+\frac{1}{2}}} j_x(x,y)dy/\Delta y_j . \tag{29}$$

Define a quantity Q(x) such that

$$Q(x)\Phi_o(x) = \frac{j_y(x,y_{j+\frac{1}{2}}) - j_y(x,y_{j-\frac{1}{2}})}{\Delta y_j} . \tag{30}$$

The leakage as a function of x on the right-hand side of Eq. (30) is assumed to come from the two-dimensional computation and thus is known. The advantage of expressing it as a product of a function and the flux is that this term is automatically scaled while the S_n code is iterating for the flux, so the correct transverse leakage is maintained. This requires that this term be placed within the source of Eq. (28), and the problem reduces to the conventional source iteration. This method thereby offers a possibility of iterating the generalized diffusion technique to improve the final solution

without extensive code modifications.

Another attractive possibility for obtaining accurate trial solutions is to use Cobb's synthesis approach.[7] Briefly, the method is to assume an expansion of the angular flux as

$$\phi(x,y,\mu,\eta) = \sum_{k=1}^{K} \psi_k(x) a_k(y,\mu,\eta), \qquad (31)$$

where $\psi_k(x)$ is a trial solution through the k^{th} region and $a(y,\mu,\eta)$ is the unknown. The equation developed for a_k is a transport equation in one dimension and two angles. This modal approach has the advantage of using a self-contained iteration to obtain a transport estimate of the flux for the entire system. Together with Eq. (31), this yields a two-dimensional approximation to the transport flux. However, this expression can also be integrated over selected regions and used as trial solutions for the generalized diffusion equation method to attain increased accuracy and reliability of solution. If this and other appropriate methods are used to improve the trial solution computation, versatility and increased applicability of the method for computing the multidimensional neutron flux of a given system result.

The theoretical analysis of the generalized diffusion method should be pursued to gain further insight on improvements in adapting it to realistic problems in particle transport. For example, if methods could be developed for one-dimensional S_n transport to choose a mesh to ensure that the quantity F_i of Eq. (13) remains positive for the trial solution, then some of the practical difficulties in using the method would be avoided. Also, a more exact statement of the effect of the trial solution on the accuracy of the generalized diffusion solution is desirable. It is particularly important to be able to show under what conditions the generalized diffusion solution lies between the transport and conventional diffusion solution.

The generalized diffusion method is presently useful for analysis of a large variety of reactor-type systems including shields, and it should be experimented with more widely. The method promises more versatility than existing methods that couple multidimensional diffusion theory with selected transport "fixes" of cross sections to account for regions where diffusion theory is inapplicable.

REFERENCES

1. K. D. Lathrop and F. W. Brinkley, "Theory and Use of the General-Geometry TWØTRAN Program," LASL report LA-4432 (1970).

2. Bengt G. Carlson and Kaye D. Lathrop, "Transport Theory, The Method of Discrete Ordinates," LASL report LA-3251-MS (1965).

3. Raymond E. Alcouffe, "A Study of Two-Dimensional S_n Transport Synthesis Via 'Angle Collapse'," Trans. Amer. Nucl. Soc. 14, 217 (1971).

4. M. Natelson, "A Strategy for the Application of Space-Angle Synthesis to Practical Problems in Neutron Transport," Nucl. Sci. Eng. 31, 325-336 (1968).

5. Raymond E. Alcouffe, Thomas J. Hirons, and R. Douglas O'Dell, "Effect of Collapsing Cross Section Data or Fast Breeder Physics Parameters," Nucl. Sci. Eng. 43, 173-185 (1971).

6. Raymond E. Alcouffe and Thomas J. Hirons, "The Effect of Condensing the Spatial Mesh on the Accuracy of Fast Breeder Fuel-Cycle Analysis," Nucl. Sci. Eng. 45, (1971).

7. William Ronald Cobb, "Application of Variational Synthesis to Solutions of Multidimensional Neutron Transport Problems," (Thesis), Oak Ridge National Laboratory report ORNL-TM-3200 (1971).

APPENDIX

DERIVATION OF THE DIFFUSION EQUATION FROM THE NEUTRON-TRANSPORT EQUATION

The stationary linear Boltzmann equation for neutron transport is written as

$$\underline{\Omega}\cdot\nabla\phi(\underline{r},\underline{\Omega},E) + \Sigma_T(\underline{r},E)\phi(\underline{r},\underline{\Omega},E)$$

$$-\int d\underline{\Omega}'\int dE'\ \Sigma_s(\underline{r},\mu_o,E'\to E)$$

$$\cdot\ \phi(\underline{r},\underline{\Omega}',E') - S(\underline{r},\underline{\Omega},E) = 0\ , \qquad \text{(A1)}$$

where $\mu_o = \underline{\Omega}\cdot\underline{\Omega}'$ and the other terms have their conventional interpretation. Integrate Eq. (A1) over $\underline{\Omega}$ to obtain

$$\nabla\cdot J(\underline{r},E) + \Sigma_T(\underline{r},E)\phi_o(\underline{r},E)$$

$$-\int_o^\infty \Sigma_{so}(\underline{r},E'\to E)\phi_o(\underline{r},E')dE'$$

$$- S_o(\underline{r},E) = 0\ , \qquad \text{(A2)}$$

where

$$\phi_o(\underline{r},E) = \frac{1}{4\pi}\int\phi(\underline{r},\underline{\Omega},E)d\underline{\Omega}\ ,$$

$$\underline{J}(\underline{r},E) = \frac{1}{4\pi}\int\underline{\Omega}\phi(\underline{r},\underline{\Omega},E)d\underline{\Omega}\ ,$$

$$\Sigma_{so}(\underline{r},E'\to E) = \int d\underline{\Omega}\Sigma_s(\underline{r},\mu_o,E'\to E)\ .$$

If the first moment of Eq. (A1) with respect to $\underline{\Omega}$ is also taken,

$$\nabla\cdot\underline{\underline{P}}(\underline{r},E) + \Sigma_T(\underline{r},E)\ \underline{J}(\underline{r},E)$$

$$-\int_o^\infty dE'\Sigma_{s1}(\underline{r},E'\to E)\underline{J}(\underline{r},E')$$

$$-\ \underline{S}_1(\underline{r},E) = 0\ , \qquad \text{(A3)}$$

where

$$\underline{\underline{P}}(\underline{r},E) = \int d\underline{\Omega}\ \underline{\Omega}\ \underline{\Omega}\ \phi(\underline{r},\underline{\Omega},E) \quad \text{(a diad)}\ ,$$

$$\Sigma_{s1}(\underline{r},E'\to E) = \int d\underline{\Omega}P_1(\mu_o)\ \Sigma_s(\underline{r},\mu_o,E'\to E)\ .$$

The diffusion approximation results if Eq. (A3) is used to define the current $\underline{J}(\underline{r},E)$. To do this, the following approximation is made in Eq. (A3).

$$\phi(\underline{r},\underline{\Omega},E) \simeq \phi_o(\underline{r},E) + \underline{\Omega}\cdot\underline{J}(\underline{r},E),$$

$\therefore$ the quantity $\underline{\underline{P}}(\underline{r},E) = \frac{1}{3}\underline{\underline{I}}\ \phi_o(\underline{r},E)$ where $\underline{\underline{I}}$ is the unit diad. Also asssume that

$$\Sigma_{s1}(\underline{r},E'\to E) = \Sigma_{s1}(\underline{r},E')\ \delta(E'\to E)\ . \qquad \text{(A3.b)}$$

With these assumptions, Eq. (A3) becomes

$$\frac{1}{3}\nabla\phi_o(\underline{r},E) + \Sigma_T(\underline{r},E)\ \underline{J}(\underline{r},E)$$

$$-\Sigma_{s1}(\underline{r},E)\underline{J}(\underline{r},E) = \underline{S}_1(\underline{r},E),$$

or

$$\underline{J}(\underline{r},E) =$$

$$-\frac{1}{3[\Sigma_T(r,E) - \Sigma_{s1}(\underline{r},E)]}\left[\nabla\phi_o(\underline{r},E) - \underline{S}_1(\underline{r},E)\right]. \qquad \text{(A4)}$$

Equation (A4) is a statement of Fick's law relating the gradient of the flux to the current, with the proportional quantity, the diffusion coefficient, given by $D(\underline{r},E) = \frac{1}{3\Sigma_{Tr}(\underline{r},E)}$ with the transport cross section $\Sigma_T\ (\underline{r},E) = \Sigma_T(\underline{r},E) - \Sigma_{s1}(\underline{r},E)$. Substituting Eq. (A4) into Eq. (A2) gives the conventional diffusion equation

$$-\nabla\cdot D(\underline{r},E)\nabla\phi_o(\underline{r},E) + \Sigma_T(\underline{r},E)\phi_o(\underline{r},E)$$

$$=\int_o^\infty dE'\Sigma_{so}(\underline{r},E'\to E)\phi_o(r,E')$$

$$+\ S_o(\underline{r},E) - \nabla\cdot D(\underline{r},E)\ \underline{S}_1(r,E)\ . \qquad \text{(A5)}$$

The assumption that $\underline{\underline{P}}(\underline{r},E)\propto \underline{\underline{I}}\ \phi_o(\underline{r},E)$ is the most severe of those necessary to derive the diffusion equation. One is essentially ignoring the higher order moments of the flux and hence assuming that the flux is a slowly varying function of angle through space and energy. This is generally true if the flux is evaluated far from the boundaries of strong absorbers or sources and far from vacuum boundaries.

The applicability of the diffusion equation form can be generalized by making, instead of the assumption of Eq. (A3.b), the assumption that

$$\underline{J}(\underline{r},E) = - \underline{\underline{D}}(\underline{r},E) \cdot \nabla\phi_o(\underline{r},E)$$

where the diad $\underline{\underline{D}}$ is defined by

$$D_{ij}(\underline{r},E) = - \frac{\underline{J}(\underline{r},E) \cdot \hat{\underline{\ell}}_i}{\nabla\phi_o(\underline{r},E) \cdot \hat{\underline{\ell}}_i} \text{ for } i=j=1,2,3 \qquad (A6)$$

$$= 0 \text{ for } i \neq j.$$

In this case Eq. (2) becomes

$$- \nabla \cdot \underline{\underline{D}}(\underline{r},E) \cdot \nabla\phi_o(\underline{r},E) + \Sigma_T(\underline{r},E)\, \phi_o(\underline{r},E)$$

$$- \int_o^\infty \Sigma_{so}(\underline{r},E' \to E)\phi_o(\underline{r},E')\, dE'$$

$$= S_o(\underline{r},E) \qquad (A7)$$

For boundary conditions consistent with the transport equation, the solution to Eq. (A7) will reproduce the angle integrated transport flux. The numerical analog to this procedure is used to derive the generalized diffusion equation of Section II.