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ABSTRACT

Current work and trends in the application of neutron diffusion theory to reactor design and analysis are reviewed. Specific topics covered include finite-difference methods, synthesis methods, nodal calculations, finite-elements and perturbation theory.

INTRODUCTION

The analysis of nuclear reactor cores is dominated by two fundamental concerns. In somewhat oversimplified terms, the first is finding where the neutrons are and what they are doing. The second is determining criticality, the state of the core that is required in order to sustain the fission chain reaction. Among the various deterministic and probabalistic methods available for treating these problems neutron diffusion theory is by far the most widely used.

The distribution of neutrons is most conveniently described by the scalar neutron flux, $\phi(\bar{x},E,t)$, which, in general, is a function of space ($\bar{x}$), energy (E) and time (t), and which is the product of the neutron speed, v(E), and the neutron population density, $n(\bar{x},E,t)$. Given the flux and cross sections (the probabilities per unit flux of neutrons interacting in various ways with the nuclei of atoms forming the materials in a reactor) one may directly determine heat generation rates, neutron radiation exposures, fuel burnup, and other quantities which affect the performance, safety and economy of nuclear reactors.

With deterministic methods of reactor analysis the energy variable is almost always treated with multigroup theory. The continuous neutron energy spectrum is replaced by a set of G energy groups,

$$\begin{array}{ccc} \phi(\bar{x},E,t) & \rightarrow & \phi^g(\bar{x},t) \quad , \\ 0 \le E < \infty & & 1 \le g \le G \end{array} \qquad (1)$$

and cross sections for reactions resulting in changes in neutron energy are defined in terms of transfers from one group to another. One or two energy groups suffice for most thermal reactor design calculations; the limiting factor is the fine structure of the spatial distribution. On the order of ten-group calculations are common in fast reactor design, where the analysis is very sensitive to the energy dependence of cross sections. More energy groups, perhaps twenty or thirty, are used for the analysis of effects that are particularly sensitve to the neutron spectrum (e.g. reactivity coefficients for safety calculations).

Since the subject of this review is diffusion theory, and not reactor kinetics, we will drop the time dependence of the flux. Most methods of treating the spatial dependence of the flux can be extended to include time dependence without introducing serious theoretical complications. This review will concentrate on several current areas of interest in applications of diffusion theory to multidimensional (two-dimensional and three-dimensional) static calculations.

THE MULTIGROUP DIFFUSION EQUATIONS

With the preceding simplifications the multigroup neutron diffusion equations for a critical system can be written either as a second-order partial differential equation,

$$- \bar{\nabla} \cdot (D(\bar{x})\ \bar{\nabla} \phi\ (\bar{x})) + (A(\bar{x}) - \frac{1}{k} M(\bar{x}))\ \phi(\bar{x}) = 0, \tag{2}$$

or in the P_1 form,

$$\bar{\nabla} \cdot \bar{J}(\bar{x}) + (A(\bar{x}) - \frac{1}{k} M(\bar{x}))\ \phi(\bar{x}) = 0, \tag{3a}$$

$$\bar{J}(\bar{x}) + D(\bar{x})\ \bar{\nabla}\phi(\bar{x}) = 0. \tag{3b}$$

$\phi(\bar{x})$ is a vector of group fluxes whose elements are $\phi^g(\bar{x})$. $\bar{J}(\bar{x})$ is the neutron current, whose three spatial components $J^x(\bar{x})$, $J^y(\bar{x})$ and $J^z(\bar{x})$ (each a group vector like the flux) are the net flow of neutrons per unit area and time in each group in the x, y and z directions. k is the eigenvalue. In principle k should be 1.0 for a model of a critical reactor; in practice inadequacies in the modeling procedures lead to "critical eigenvalues" on the order of .01 different from unity for models of cores and critical assemblies known to be critical.

$A(\bar{x})$, $M(\bar{x})$ and $D(\bar{x})$ are GxG matrices. The elements of $A(\bar{x})\ \phi(\bar{x})$ are the net losses of neutrons in each group due to absorption and group-to-group scattering transfers. The elements of $M(\bar{x})\ \phi(\bar{x})$ are the net sources of fission neutrons in each group. $D(\bar{x})$ is a diagonal matrix of diffusion coefficients; in isotropic materials

$$D(\bar{x}) = (3\ \Sigma^{g}_{tr}(\bar{x}))^{-1}, \tag{4}$$

where $\Sigma^{g}_{tr}(\bar{x})$ is the transport cross section.

At internal boundaries in the region of solution of Eqs. (2) and (3) both fluxes and currents must be continuous. At the outer boundaries of the region of solution the boundary conditions are usually either homogeneous or periodic. The homogeneous form is

$$a^{g}\ \phi^{g}(s) + b^{g}\ \hat{n} \cdot \bar{J}^{g}(s) = 0. \tag{5}$$

a^{g} and b^{g} are scalar constants (one of them may be zero). s denotes the outer surface and $\hat{n}$ is the unit normal to that surface. Periodic boundary conditions require that the flux and current along one boundary of the model match those along another and are used, when the symmetry of the problem permits, to reduce the size of the region of solution.

Eq. (3b) is "Fick's law" and is a fundamental feature of all applications of diffusion theory (e.g. heat conduction). Useful corollaries to Fick's law are expressions for the partial neutron currents, the flow of neutrons, per unit area and time, in the positive (+) and negative (-) directions for each coordinate (d).

$$J^{d+}(\bar{x}) = \frac{1}{4}\,\phi(\bar{x}) + \frac{1}{2}\,J^{d}(\bar{x}), \tag{6a}$$

$$J^{d-}(\bar{x}) = \frac{1}{4}\,\phi(\bar{x}) - \frac{1}{2}\,J^{d}(\bar{x}), \tag{6b}$$

$$J^{d}(\bar{x}) = J^{d+}(\bar{x}) - J^{d-}(\bar{x}), \qquad d = x,y,z. \tag{6c}$$

In practical applications few attempts are ever made to solve the differential forms of the diffusion equations (Eqs. (2) and (3)). A variety of approximations are usually employed, and a third form, the so-called weak form, of the diffusion equation is often used to provide a formalism for developing these approximate methods. Consider the functional,

$$F = \sum_{r} \int_{r} d\bar{x} \left[\psi^*(\bar{x}) \; (A(\bar{x}) - \frac{1}{k}\, M(\bar{x}))\; \psi(\bar{x}) \right.$$
$$\left. + \,\bar{\nabla}\, \psi^*(\bar{x}) \cdot D(x)\; \bar{\nabla}\, \psi(\bar{x}) \right]. \tag{7}$$

The subscript r denotes regions where the material properities of the reactor model are continuous. The vectors $\psi^*(\bar{x})$ and $\psi(\bar{x})$ are arbitrary "trial functions."

When one requires that the change in the value of F (the variation of F) due to arbitrary, independent and infinitesimal changes to the trial functions ($\delta\psi^*(\bar{x})$ and $\delta\psi(\bar{x})$) be zero,

$$\begin{aligned}\delta F = 0 = \sum_r \int_r d\bar{x}\ \delta\psi^*(\bar{x}) & \left[(A(\bar{x}) - \frac{1}{k} M(\bar{x}))\ \psi(\bar{x}) - \bar{\nabla} \cdot D(\bar{x})\ \bar{\nabla}\ \psi(\bar{x})\right] \\ + \sum_r \int_r dx\ \delta\psi(\bar{x}) & \left[(A^T(\bar{x}) - \frac{1}{k} M^T(\bar{x}))\ \psi^*(\bar{x}) - \bar{\nabla} \cdot D^T(\bar{x})\ \bar{\nabla}\ \psi^*(\bar{x})\right] \\ + \sum_s \int_s ds\ \delta\psi^*(s) & \left[D(s-)\ \hat{n} \cdot \nabla\psi(s-) - D(s+)\ \hat{n} \cdot \nabla\psi(s+)\right] \\ + \sum_s \int_s ds\ \delta\psi(s) & \left[D^T(s-)\ \hat{n} \cdot \nabla\psi^*(s-) - D^T(s+)\ \hat{n} \cdot \nabla\psi^*(s+)\right] .\end{aligned} \tag{8}$$

s denotes the internal boundaries between regions; the signs (+) and (-) distinguish the two sides of each interface. When the variations permitted to the trial functions are completely arbitrary the condition, $\delta F = 0$, implies that $\psi(\bar{x})$ satisfies Eq. (2) and the current continuity condition. The additional Euler equations for $\psi^*(\bar{x})$ introduce the adjoint flux, $\phi^*(\bar{x})$, which is defined by,

$$- \bar{\nabla} \cdot (D^T(\bar{x})\ \bar{\nabla}\ \phi^*(\bar{x})) + (A^T(\bar{x}) - \frac{1}{k} M^T(\bar{x}))\ \phi^*(\bar{x}) = 0. \tag{9}$$

A variety of approximate solutions to the diffusion equation may be derived by substituting particular trial solutions (each with a limited number of undetermined parameters) into Eq. (7) and requiring $\delta F = 0$. In these cases the variations to the trail functions, $\delta\psi^*(\bar{x})$ and $\delta\psi(\bar{x})$, are no longer completely arbitrary, and the trial functions will not, in general, satisfy the differential forms of the diffusion equation everywhere in the region of solution. Equation (8) is a weaker statement of the neutron balance than Eqs. (2) and (3).

Note that it is not necessary for the trail solutions to produce continuous currents at internal boundaries as long as $\delta\psi^*(s)$ is not identically zero. Continuity of flux can be guaranteed either by supplying continuous trial functions or by adding surface terms to the functional (Eq. (7)) that lead to additional Euler equations establishing continuity of flux. Several functionals that explicitly permit discontinuous trial functions have been discussed in papers by Stacey(1) and Nelson.(2) In addition to the form shown in Eq. (7) functionals can be written which yield the P_1 equations and which permit separate trial functions for flux and current.

THE FINE-MESH, FINITE-DIFFERENCE EQUATIONS

To adapt the diffusion equation to digital computers the continuous, differential forms of Eqs. (2), (3) and (7) must be converted to discrete representations. The most direct approach, the "fine-mesh, finite-difference" approximation, leads to a set of linear, coupled algebraic equations. One- and two-dimensional, finite-difference calculations have long been a staple of reactor design. In recent years finite-difference codes for three-dimensional calculations have become available and are becoming important tools in reactor analysis. Among them are PDQ-7(3), TRITON(4), 3DB(5) and VENTURE(6).

The first step in any discretization of the diffusion equation is the superposition of a grid, or mesh structure, on the region of solution. Figure 1 shows a few "mesh cells" of such a structure for a two-dimensional, x-y geometry. I+1 vertical and J+1 horizontal mesh lines divide the model into IxJ mesh cells, each homogeneous in composition. Mesh cell (i,j) is bounded by vertical lines at $x = x_{i-1}$ and $x = x_i$ and by horizontal lines at $y = y_{j-1}$ and $y = y_j$. The four outer boundaries of the region of solution are $x = x_0$, $x = x_I$, $y = y_0$ and $y = y_J$.

Two forms of the fine-mesh, finite-difference, diffusion theory equations are in widespread use: the "corner-mesh" equations$^{(7,8)}$ and the "mesh-centered" equations$^{(5,6)}$. The derivations of both forms are based on Taylor series expansions of the flux within a small volume, a neutron balance within that volume, and the imposition of average flux and current continuity at the boundaries of the volume. When the volume boundary lies on the external boundary of the region of solution, the external boundary conditions (e.g. Eq. (5)) are used instead of the continuity conditions.

For the corner-mesh form, and for the two-dimensional geometry shown in Fig. 1, the neutron balance (Eqs. (2) or (3a)) is integrated over the area defined by the dashed lines. The dashed lines bisect, at right angles, the mesh line segments connecting the intersection of lines $x = x_i$ and $y = y_j$ (point "a") to the next nearest intersections along each mesh line. For the mesh-centered form the flux is expanded about the center of each mesh cell (point "b" in Fig. 1). For either approach to the discretization the final form of the finite-difference equations may be written,

$$\begin{aligned} &\gamma^x_{ij}(\phi_{ij} - \phi_{i-1j}) - \gamma^x_{i+1j}(\phi_{i+1j} - \phi_{ij}) + \\ &\gamma^y_{ij}(\phi_{ij} - \phi_{ij-1}) - \gamma^y_{ij+1}(\phi_{ij+1} - \phi_{ij}) + \qquad (10) \\ &\alpha_{ij}\,\phi_{ij} = 0. \end{aligned}$$

Fig. 1. A portion of a two-dimensional mesh structure. Mesh cell (i,j) is bounded by vertical mesh lines at $x = x_{i-1}$ and $x = x_i$ and by horizontal mesh lines at $y = y_{j-1}$ and $y = y_j$. The dashed lines define a neutron balance volume about point "a" for the corner-mesh form of the finite-difference equations. The mesh-centered form of the equations derives from a balance in mesh cell (i,j) about point "b".

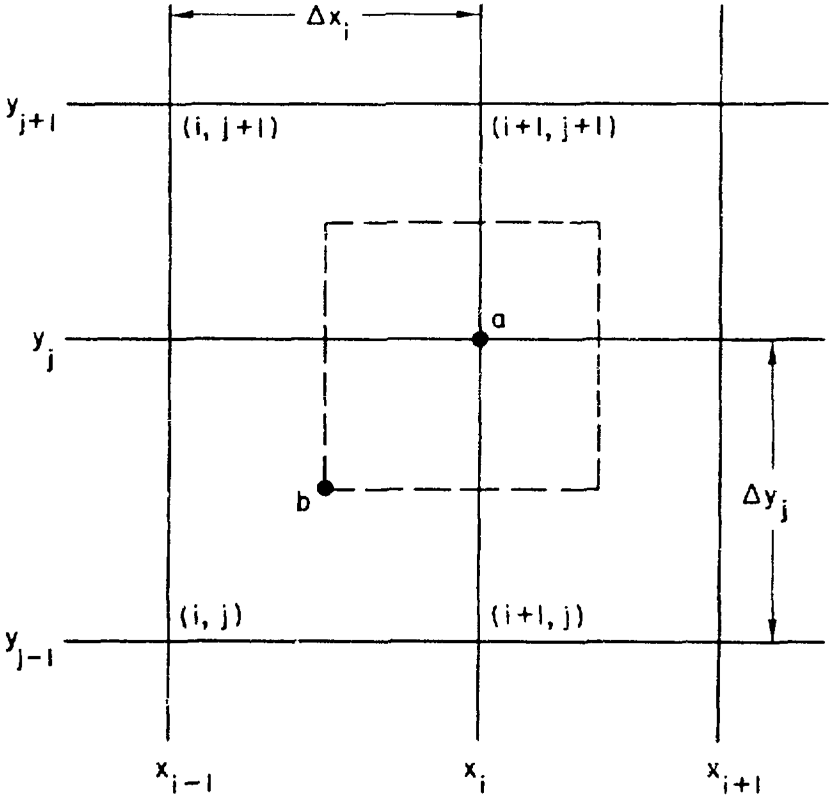
Δx_i
y_{j+1}
$(i, j+1)$
$(i+1, j+1)$
a
y_j
b
Δy_j
(i, j)
$(i+1, j)$
y_{j-1}
x_{i-1}
x_i
x_{i+1}

Table I gives expressions for some of the matrix coefficients in Eq. (10). ϕ_{ij} is the zero order Taylor series term and, therefore, can be interpreted as the flux at point "a" or point "b" for the corner-mesh and mesh-centered differencing schemes, respectively. γ^y_{ij} for interior mesh points, and γ^x_{ij} and γ^y_{ij} on boundaries other than $x = x_0$ may be obtained from Table I by switching x and y coordinates and/or reversing the indexing.

For Eq. (10) to be valid on the boundaries of the region of solution certain conventions of notation must be observed. Point fluxes (ϕ_{ij}) outside the region of solution (e.g. ϕ_{-1j} in the corner-mesh equations for $i = 0$ and ϕ_{0j} in the mesh-centered equations for $i = 1$) are identically zero for boundary conditions of the type shown in Eq. (5). Along a boundary with periodic conditions, point fluxes outside the region of solution are identical to point fluxes within the region of solution along another boundary.

When working with the differential form of the diffusion equations one must consider not only the neutron balance (Eqs. (2) or (3)) but also the separate equations defining the boundary conditions and flux and current continuity. No such separate side conditions are required for the finite-difference form; the boundary and continuity conditions have been absorbed into the balance equation (Eq. (10)) during the derivation.

For any practical problem, even in one dimension, it is not feasible to solve the matrix eigenvalue problem (Eq. (10)) directly. Computer codes are structured as a series of "outer iterations". Each outer iteration is a solution of an inhomogeneous equation that results when some of the terms in Eq. (10) are collected together and evaluated using fluxes and eigenvalue estimates from previous iterations. In one dimension it is often possible to solve each inhomogeneous calculation directly; in two and three dimensions each inhomogeneous solution must be done iteratively, through a series of "inner iterations".

TABLE I. Definitions of Some of the X-Y Geometry, Finite-Difference Coefficients in Eq. (10). In the Expressions for $\alpha^{gg'}_{ij}$, $\Sigma^{gg'}_{ij} = A^{gg'}_{ij} - \frac{1}{k} M^{gg'}_{ij}$

	corner-mesh equations	mesh-centered eequations
γ^{xg}_{ij} at internal mesh points	$\frac{D^g_{ij}\Delta y_j + D^g_{ij+1}\Delta y_{j+1}}{2\Delta x_i}$ i=1...I j=1...J-1	$\frac{2D^g_{i-1j}D^g_{ij}\Delta y_j}{\Delta x_i D^g_{i-1j} + \Delta x_{i-1} D^g_{ij}}$ i=2...I j=1...J
$\alpha^{gg'}_{ij}$ at internal mesh points	$\frac{1}{4}(\Delta x_i \Delta y_j\ \Sigma^{gg'}_{ij} + \Delta x_{i+1}\Delta y_j\ \Sigma^{gg'}_{i+1j}$ $+ \Delta x_i \Delta y_{j+1}\ \Sigma^{gg'}_{ij+1} + \Delta x_{i+1}\Delta y_{j+1}\ \Sigma^{gg'}_{i+1j+1})$ i=1...I-1 j=1...J-1	$\Delta x_i \Delta y_j\ \Sigma^{gg'}_{ij}$ i=1...I j=1...J
γ^{xg}_{ij} at x = x_0 boundary	$\frac{a^g}{b^g}\ \frac{\Delta y_j + \Delta y_{j+1}}{2}$ i=0 j=1...J-1	$\frac{D^g_{ij}a^g\Delta y_j}{D^g_{ij}b^g + \frac{1}{2}\Delta x_i a^g}$ i=1 j=1...J

The theory behind the iterative techniques used to solve the finite-difference equations is well established$^{(7-9)}$, but codes differ somewhat in how they apply the available acceleration procedures. For example, PDQ-7$^{(3)}$, which has become something of a standard in light-water reactor design, uses Chebyshev polynomials on the group fluxes to accelerate the convergence of the outer, power iterations. Ferguson and Derstine, in a paper at this meeting,$^{(10)}$ show that for fast reactor applications significant improvements in efficiency can be achieved by using a very similar strategy with Chebyshev acceleration of the fission source.

Finally, as in the case of the continuous form, one can write a weak form of the finite-difference, diffusion theory equations. The following functional, subject to the conventions and definitions defined earlier, will yield Eq. (10) as its Euler equation.

$$\begin{aligned} F = &\sum_{ij} (\phi^*_{ij} - \phi^*_{i-ij})\, \gamma^x_{ij} (\phi_{ij} - \phi_{i-1j}) \\ &+ \sum_{ij} (\phi^*_{ij} - \phi^*_{ij-1})\, \gamma^y_{ij} (\phi_{ij} - \phi_{ij-1}) \qquad (11) \\ &+ \sum_{ij} (\phi^*_{ij}\, \alpha_{ij}\, \phi_{ij} . \end{aligned}$$

Although a variety of mesh geometries (e.g. x-y-z, r-z, triangular) are treated by available codes, most involve low-order, nearest-neighbor coupling schemes comparable to Eq. (10) and Table I. Abu-Shumays and Hageman$^{(11)}$ have derived a number of higher-order finite-difference equations for regular mesh arrays, but at a cost of a more complicated coupling. They also have derived finite-difference equations for an arbitrary, quadrilaterial mesh, that is, one for which the mesh lines are not all parallel. Natelson et al.$^{(12)}$ have varied the mesh with energy group.

Existing codes on the current generation of computers permit two-dimensional, fine-mesh finite difference calculations on a more or less routine bases. We have not yet reached the point, however, where routine fine-mesh, design calculations can be carried out in three dimensions. Accurate fine-mesh models call for mesh spacings of a few centimeters or less, and in three dimensions this requirement translates into hundreds of thousands of space-energy points. This limitation is felt in both thermal reactor calculations, where the diffusion length for neutrons may be on the order of a centimeter, as well as fast reactor calculations, where the diffusion length is significantly longer but the number of energy groups is greater. The advent of faster computers with larger fast memories will make three-dimensional fine-mesh calculations more practical. Vector processing capabilities may prompt the development of new iteration strategies.

SYNTHESIS METHODS

Although reactor models are always heterogeneous, they are frequently "less heterogeneous" in one direction than in the others. Along lines parallel to fuel elements or coolant channels one encounters few material discontinuities, and the neutron flux is relatively slowly varying. For all practical purposes, the flux may be treated as separable over all, or at least part, of the region of solution. Under these conditions synthesis methods may be used to combine several, local solutions of the diffusion equation into a single, global one.

The separability of the three-dimensional neutron flux into axial and planar factors is implicit in every two-dimensional, planar calculation which uses a buckling to approximate the axial leakage. The term synthesis is never applied to this practice, but, in fact, the three-dimensional equations have been reduced to two dimensions by factoring the flux,

$$\phi^g_{(x,y,z)} \rightarrow a^g_{(x,y,z)}\ \phi^g_{(x,y)}, \tag{12}$$

and introducing a buckling.

$$\frac{\partial}{\partial z} D^g_{(x,y,z)} \frac{\partial}{\partial z} a^g_{(x,y,z)} = - D^g_{(x,y,z)} (B^2_{(x,y,z)})^g\ a^g_{(x,y,z)} \tag{13}$$

$$\frac{\partial}{\partial z} D^g_{(x,y,z)} \frac{\partial}{\partial z} \phi^g_{(x,y,z)} \rightarrow - D^g_{(x,y,z)} (B^2_{(x,y,z)})^g\ \phi^g_{(x,y,z)} \tag{14}$$

In practice bucklings, $(B^2_{(x,y,z)})^g$, are chosen either arbitrarily (presumably on the basis of some prior knowledge of the axial shape of the flux) or by iteration within the two-dimensional calculation. The iterative procedure usually requires a space- and energy independent buckling, B^2, and the goal is to adjust B^2 so that the eigenvalue of the two-dimensional calculation matches the "critical eigenvalue" expected for the three-dimensional problem.

The codes BISYN(13) and SYNBURN(14) extend the buckling approximation towards an automated synthesis scheme for two-dimensional models by alternating one-dimensional calculations in the two different directions. Transverse leakages are approximated by bucklings which are updated after each one-dimensional solution. Three-dimensional calculations, which alternate one- and two-dimensional calculations, have also been tested(15). It is not clear from published results how accurate these methods are near core-reflector or core-blanket interfaces, where the reduced equations may contain large, negative bucklings.

The single-channel and multichannel spatial flux synthesis approximations provide a determination of the axial shape factor in a more direct way.(1,16,17) One starts with a set of precalculated, fine-mesh finite-difference, two-dimensional flux solutions, ψ^g_{nij} $(n = 1...N)$, which represent the best practical estimates of the planar flux shapes at a number of axial locations. In the basic, single-channel flux synthesis approximation the three-dimensional flux, ϕ^g_{ijk}, is assumed to be a blend of these two-dimensional expansion functions,

$$\phi^g_{ijk} = \sum_{n=1}^{N} A^g_{nk} \psi^g_{nij} . \tag{15}$$

For those energy groups, g, or axial positions, k, where a particular expansion function, ψ_n, cannot be expected to make a useful contribution to the three-dimensional, synthesized flux (Eq. (15)) it may be "turned off" by the simple device of defining the combining coefficient, A^g_{nk}, to be identically zero.

Equation (15) is written in terms of the discrete form of the neutron flux. This was done because, as a practical matter, the expansion functions for synthesis calculations must be generated in the discrete form by finite-difference methods (Eq. (10)). Although many derivations of the synthesis equations in the literature are written in terms of the continuous form of the diffusion equations, a more consistent approach is to work entirely in the discrete representation. This can be done by substituting Eq. (15) into the weak form of the finite-difference, diffusion theory equation (Eq. (11)) and then setting the variations of F with respect to the non-zero combining coefficients equal to zero. The usual practice is to use the same expansion functions, ψ^g_{nij}, for the direct and adjoint synthesis expansion.

Working strictly in the discrete form is not only consistent with the nature of the expansion functions, it also avoids the problems of dealing with continuity and boundary conditions that must be faced with the continuous form. Discontinuous trial functions are handled automatically by Eq. (11); the boundary and continuity conditions are implied in the finite-difference coefficients.

The basic multichannel spatial flux synthesis approximation can be written,

$$\phi^g_{ijk} = \sum_{n=1}^{N} \sum_{c=1}^{C_n} A^g_{nck}\ f^g_{ncij}\ \psi^g_{nij}, \tag{16}$$

which differs from Eq. (15) by the additional sum over index c (for channel) and the set of multichannel basis functions f^g_{ncij}, which permit some modulation of the original expansion functions. In the original work by Washspress and Becker(18) the basis functions were unity over a portion of the plane (a channel) and zero elsewhere. Later authors have used low order polynomials in order to make the modulations less abrupt.(19-21) Note that Eq. (16) permits different sets of basis functions for the different expansion functions.

Coarse-mesh rebalancing,(22,23) which is a method sometimes used to accelerate discrete diffusion and transport calculations, resembles multichannel synthesis. Coarse-mesh rebalancing equations can be derived in a manner similar to the synthesis method by applying a set of three-dimensional basis functions, f^g_{cijk}, to a single, three-dimensional expansion function (a partially converged solution), ψ^g_{ijk}.

$$\phi^g_{ijk} = \sum_{c=1}^{C} A^g_c\ f^g_{cijk}\ \psi^g_{ijk} \tag{17}$$

The hope is that when the combining coefficients are determined and Eq. (17) evaluated the results (ϕ^g_{ijk}) will be closer to the true solution than the original expansion function (ψ^g_{ijk}). Compared to other acceleration techniques, coarse-mesh rebalancing has a relatively weak theoretical base.

The choice of basis functions for multichannel synthesis is arbitrary, though they should probably permit the recovery of the original expansion function from the synthesis approximation (Eq. (16)). Wachspress, for example, has developed a set of functions which, in this application, will assure continuous fluxes and permit arbitrarily shaped boundaries.(24)

Most authors refer to the functions ψ^g_{nij} as "trial functions." It would perhaps be more descriptive to call Eqs. (15) and (16), the statements of the synthesis approximations, the "trial functions." Then the term "choice of trial functions" implies not only the choice of expansion functions, ψ^g_{nij}, but also the specification of ranges in energy and axial positions where the functions are to be used (the ranges of non-zero A^g_{nck}'s) and the choices of channel structure.

The choice of trial functions is not a difficult problem for single-channel calculations. Critically buckled eigenvalue problems at various elevations of the core will provide good shapes through the core. No problems have arisen in axially discontinuous synthesis calculations,(25) where functions are used only over axial zones where they are deemed appropriate. Combining coefficients should be set equal to zero (i.e. expansion functions should be dropped) a few diffusion lengths into adjacent zones, to permit the mode to decay gradually in space.(26) In axial reflectors and low reactivity zones (e.g. fast reactor blankets), where eigenvalue problems are not appropriate, fixed source problems can provide adequate shapes.(20) Multichannel synthesis requires the additional choice of channel structure; this is a problem that has not been adequately investigated.

Single-channel synthesis codes have existed for some time,(27-31) and three are available from code centers. PDQ-7(28) and SYN3D(31) may be obtained through the Argonne Code Center, and KASY(29) is at the NEA Computer Program Library at Ispra. KASY and SYN3D do not include calculations of the expansion functions; these must be generated by some other finite-difference, diffusion theory code. When finite-difference and synthesis codes are mated, care should be taken that they both use the same finite-difference form. For example, SYN3D uses the mesh-centered form, because the code was designed to be used with the mesh-centered-equation codes used in the fast reactor community.(5,6)

Nodal synthesis methods(32-34) do not fit comfortably within the strictly finite-difference approach outlined above. The nodal coupling does not come from a unified treatment of the problem as a whole but rather from special definitions of internal boundary conditions. The effect of the nodal synthesis schemes can be achieved with Eqs. (16) and (11) by limiting the number of expansion functions to one for each channel and by choosing multichannel basis functions which do not overlap channels. Although no direct comparisons have been made of different nodal synthesis schemes, Nelson has made an attempt to compare several of the explicit treatments of discontinuous trial functions in the continuous (i.e. differential equation) form of diffusion theory.(2)

COARSE-MESH AND NODAL METHODS

Fine-mesh, finite-difference, diffusion theory calculations are both reliable and familiar, and for these reasons reactor core designers and analysts have relied heavily on them. For two- and three-dimensional models, however, finite-difference methods with mesh spacings consistent with the Taylor series flux expansion approximation implicit in Eq. (10) are expensive.

Many attempts have been made to reduce the number of unknowns (the space-energy point fluxes) by using coarser mesh spacing and appropriately defined finite-difference coefficients. These methods range in sophistication from empirical adjustments of the conventional finite-difference equations (specifically the leakage coefficient γ^d_{ij} in Eq. (10)) to involved procedures employing individual diffusion theory solutions within each mesh interval, or node. Review articles by Henry(35) and Wagner(36) outline the progress of nodal methods up to recently. A thesis by Robinson contains detailed comparisons of several of the earlier methods.(37)

Because of the variety of approaches used, coarse mesh and nodal methods defy precise classification. If there is a common theme, it is that most of the methods can be reduced to finite-difference-like equations which can be solved by existing finite-difference codes modified for the purpose. The formally exact nodal equations may be obtained by integrating Eq. (3a) over a homogeneous node; in x-y geometry, and using the index notation in Fig. 1,

$$(\mathcal{J}^x_{i+1j} - \mathcal{J}^x_{ij})\,\frac{1}{\Delta x_i} + (\mathcal{J}^y_{ij+1} - \mathcal{J}^y_{ij})\,\frac{1}{\Delta y_j}$$

$$+ (A_{ij} - \frac{1}{k}\,F_{ij})\,\phi_{ij} = 0^N. \qquad (18)$$

ϕ_{ij} is the average flux in node (i,j). $\mathcal{J}^x_{i+1j}$ is the average, x-direction neutron current normal to the mesh line at $x = x_{i+1}$ between $y = y_j$ and $y = y_{j+1}$. The thrust of all nodal methods is to find a simple but accurate relationship between the average flux in a node and the currents on its faces. In many cases it is convenient to break the currents in Eq. (18) up into incoming and outgoing components by using the partial current relationships (Eq. (6a) and (6b)).

Early methods, which neglected the shape of the flux within the node, produced equations with constant finite-difference coefficients. Later methods generally make some provision for the flux shape within the node and, as a result, introduce non-linear effects into iterative solutions. A number of authors have used approximations to a Green's function to define the nodal coupling,(38-40) and one version of the MEDIUM code uses a collison probability approach.(41) These later methods were more accurate but frequently gave poor results near the core-reflector interface in the light-water reactor models to which they were applied.

More recently developed nodal methods have focused on more accurate treatments of the flux solution within the node.(42-46) These techniques are characterized by some form of continuous, in-node solution of the diffusion equation combined with sparse coupling to adjacent nodes. The combination takes advantage of the accuracy of the finite-element method, but the resulting equations retain the finite-difference form (Eq. (10)). All of these methods have yielded power distributions with errors on the order of 1% for two-dimensional, light-water reactor test calculations with nodes the size of fuel assemblies.

Aoki and Tsuiki(42) assume that the neutron source distribution within a node can be written in a particular form (a sum of exponentials) for which the inhomogeneous diffusion equation can be solved analytically. Rewriting the analytic solution in terms of point fluxes and applying continuity conditions leads, in two dimensions, to five-point equations. The source is updated in a power iteration sequence.

The COMETA code(44) uses analytic solutions of the buckling equation within each node, and then proceeds in a similar fashion to the five-point equations. The bucklings are updated each iteration from estimates of the average currents at the node interfaces.

Bennewitz et al.(43,45) and Shober et al.(46) have developed several methods which have the common feature that the in-node, multidimensional calculation is reduced to several one-dimensional calculations (by formally integrating out the transverse dimension variables). The methods differ in the nature of the one-dimensional solutions (analytic or polynomial approximations) and the treatment of the buckling term that appears in the reduction to one dimension.

All the applications of the latest generation of nodal methods have been to light-water reactors with rectangular fuel assemblies. Most, though not all, can be easily extended to multigroup models. It is less clear how to handle the hexagonal nodes required for fast reactor calculations. Because diffusion lengths are longer in fast reactors, less sophisticated methods may be adequate.

FINITE-ELEMENT METHODS

The finite-element method was used in many other fields of engineering, particularly structural mechanics, before it was applied to neutron diffusion calculations. The basic idea is to divide a reactor model into nodes (called elements), assume a polynomial expansion trial function for the flux within the node, and apply the weak form of the diffusion equation (Eq. (8)) to reduce the problem to a set of linear algebraic equations in terms of the coefficients of the polynomials. In principle the elements can be any arbitrary shape and the polynomials of any arbitrary order. In practice the elements are usually triangles or quadrilaterals (in two dimensions), and the polynomials are of relatively low order. Complicated shapes and high order polynomials lead to dense, irregularly coupled equations which resist efficient solution techniques.

A simple, finite-element approach was used several years ago in the diffusion-theory code VARI-QUIR(47). It has only been in the last few years, however, that the method has became popular. Several authors(47-52) have studied choices of elements and polynomials and have showed that the method can yield more accurate results than finite-difference codes with fewer unknowns and equations. Published timing comparisons sometimes showed improvements of factors of 50 in running times.

Several review articles have outlined the successes and problems of finite-element diffusion theory calculations.(36,53,54) The early enthusiasm for the method was largely due to test problem comparisons between finite-difference and finite-element which did not accurately reflect the heterogeneous nature of current reactor design models. For three-dimensional design methods the finite-element method will require solutions of systems of equations much larger than those which up to now have been studied. The direct methods of solution used earlier may no longer be practical; accelerated, iterative techniques will have to be employed.(54)

Although it is possible to perform accurate calculations with large, homogeneous elements, it is not always desirable. Homogenizing fuel assemblies subject to different exposures and temperatures may change the performance of the reactor model in a significant way. Deppe and Hansen(55) have had success with elements that extend over mild discontinuities in the cross section distributions. Kavenoky and Lautard(56) have extended polynomial expansions to the cross sections as well as the fluxes, permitting spatially dependent burnup within an element. Inhomogeneous elements will cost additional computing time.

Walters and Komoriya(57) have reduced the number of equations to be solved by using different element sizes in different energy groups, and by tailoring the size of the elements to the requirements for each group.

The most serious problem faced by finite-element methods is one of identity. If it is to compete successfully with fine-mesh finite-difference calculations it will have to prove its advantage for three-dimensional models with more equations than can be handled with direct solution methods. Fine-mesh finite-difference codes with solidly based iterative strategies have been around a long time, and designers and analysists have great confidence in them. Someone will have to write a finite-element equivalent of PDQ.

On the other hand, the place for finite-element methods to make a contribution may be in coarse-node applications. Some of the best of the nodal methods(43,45,46) use finite-element techniques. These methods need ageing, and perhaps some attention to programming details, before any hard comparisons can be made.

PERTURBATION THEORY

It is probably worth while every so often to remind the reactor analysis community about perturbation theory. This is particularly true since the development of generalized perturbation theory, which has expanded the range of applications of the method beyond eigenvalue changes.

The text-book form of perturbation theory yields an expression for the change in eigenvalue due to a change in the diffusion equation coefficients. The expression, which is exact,(58) requires two flux solutions, one direct and one adjoint, of the two states (unperturbed and perturbed) of the model. Exact perturbation theory saves no computing time but does provide a way of displaying the spatial and spectral details of reactivity worths, allows insights into the mechanism of feedback and assures greater accuracy than can be obtained from the difference between two eigenvalue calculations.

When the unperturbed flux and adjoint are used, perturbation theory is only good through first order, but for small perturbations the results are still accurate. Considering the number of self-adjoint (one-energy-group) calculations that are performed by reactor designers, it is surprising that perturbation theory is not more widely used.

Generalized perturbation theory(59-64) treats changes in arbitrary, homogeneous, linear and bilinear reaction rate ratios for models described by eigenvalue problems. This class of parameters includes power fractions, instantaneous breeding ratios, delayed neutron parameters and perturbation theory expressions for reactivity worths. For fixed source diffusion theory calculations the same formalism covers changes in reaction rates (e.g. detector responses).

The VARI-1D code,(65) which performs one-dimensional, generalized diffusion perturbation theory calculations, is available through the Argonne Code Center. The FORSS System(66) will eventually do generalized perturbation calculations in up to three dimensions in diffusion theory and is currently used in a transport theory mode for cross section sensitivity analysis.

Time dependent, generalized perturbation theory is at the testing stage.(67) Kallfelz et al.(68) have treated the combination of the diffusion equation and depletion equations in a perturbation approach to burnup studies.

Like synthesis methods, perturbation theory in practice is a parasitic calculation, relying on independent codes for fluxes and adjoints. It is important, therefore, that the inner products used in the perturbation expressions be properly defined to be consistent with the discrete diffusion theory form used in the flux and adjoint calculations. For the common finite-difference form of the diffusion equations (Eq. (10)) the inner products are of the form shown in the weak form finite-difference functional (Eq. (11)). It would not be appropriate, for example, to use fluxes and adjoints interpolated from a finite-element calculation in a finite-difference perturbation theory code.

There is at least one exception to this rule. Single-channel and multichannel synthesis fluxes (Eqs. (15) or (16)) and adjoints can be used in finite-difference perturbation theory codes. The synthesis and finite-difference inner products are identical as long as the synthesis calculations are based on the finite-difference diffusion equation. One must be careful about the interpretation of the results, however. Despite the fact that the perturbation theory code takes the synthesized fluxes in finite-difference form, the code really only predicts perturbations in the <u>synthesis</u> model; the analyst must still provide appropriate flux and adjoint trial functions.

DIFFUSION EQUATION CONSTANTS

The generation of the constants used in diffusion theory calculations may be considered to be within the province of reactor physics, rather than reactor mathematics, but it is so important a step in the modeling procedure that it is worth mentioning several efforts in this area. In particular, diffusion coefficients are derived quantities, and their definition has attracted a lot of attention.

There are no theoretical or calculational problems encountered if Fick's law (Eq. (3b)) is generalized to provide different diffusion coefficients in different directions. The anisotropic nature of reactor models (particularly in the presence of streaming channels) makes it an attractive option in multidimensional diffusion theory calculations. The problem arises when one tries to choose values for directional-dependent diffusion coefficients. A number of authors (69-72) have investigated methods, and a paper at this conference describes an application to void streaming. (73) However, there does not yet appear to be a concensus on a valid approach.

Kollas and Henry (74) have derived diffusion coefficients from analytic solutions in one-dimensional slabs. Pryor and Sicilian (75) have determined diffusion coefficients by combining fine mesh diffusion theory solutions and the response matrix formalism. This is a non-linear procedure, but is one way of including transport effects in diffusion theory calculations.

Although some of the most recent nodal methods do not appear to require special treatment of interfaces, others employ special boundary conditions. The core-reflector interface has received special attention (76,77); in water-moderated reactor models this region has been especially difficult to calculate. Becker (78) has suggested power corrections to account for thermal spectrum transients near zone interfaces.

Finally, a number of authors have investigated alternative methods of group collapsing cross sections, several of which fall into the category of spectral synthesis. Kiguchi (79) has derived a sort of modified one-group method based on spectral synthesis for the case when one spectral mode can be expected to dominate. Salvatores (80) and Wade and Bucher (81) have looked at various adjoint weighting schemes. In a paper at this conference Nelson (82) considers some theoretical aspects of spectral synthesis.

SUMMARY

The most powerful tool of reactor analysis and design is, and will probably remain, the finite-difference form of the neutron diffusion equation. Detailed spatial calculations are currently performed, at a significant cost, for reactor core models with hundreds of thousands of space-energy points. Reactor plant simulators with fast-running, coarse-mesh finite-difference calculations are used routinely for a variety of design calculations where the requirements of accuracy are not too severe.

Among the alternatives for diffusion theory calculations the nodal methods have made the greatest progress in recent years. Synthesis methods are used sparingly; suspicion of their behavior and the inconvenience of the extra work required in generating expansion functions seem to discourage potential users. Finite-element methods are fast and accurate, but finite-element codes are not generally available; solution techniques for the finite-element equations need more attention.

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