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Test of the Diffusion Theory Difference Equations in Slab Geometry (Computer Code VANCER)

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D. R. Vondy and T. B. Fowler

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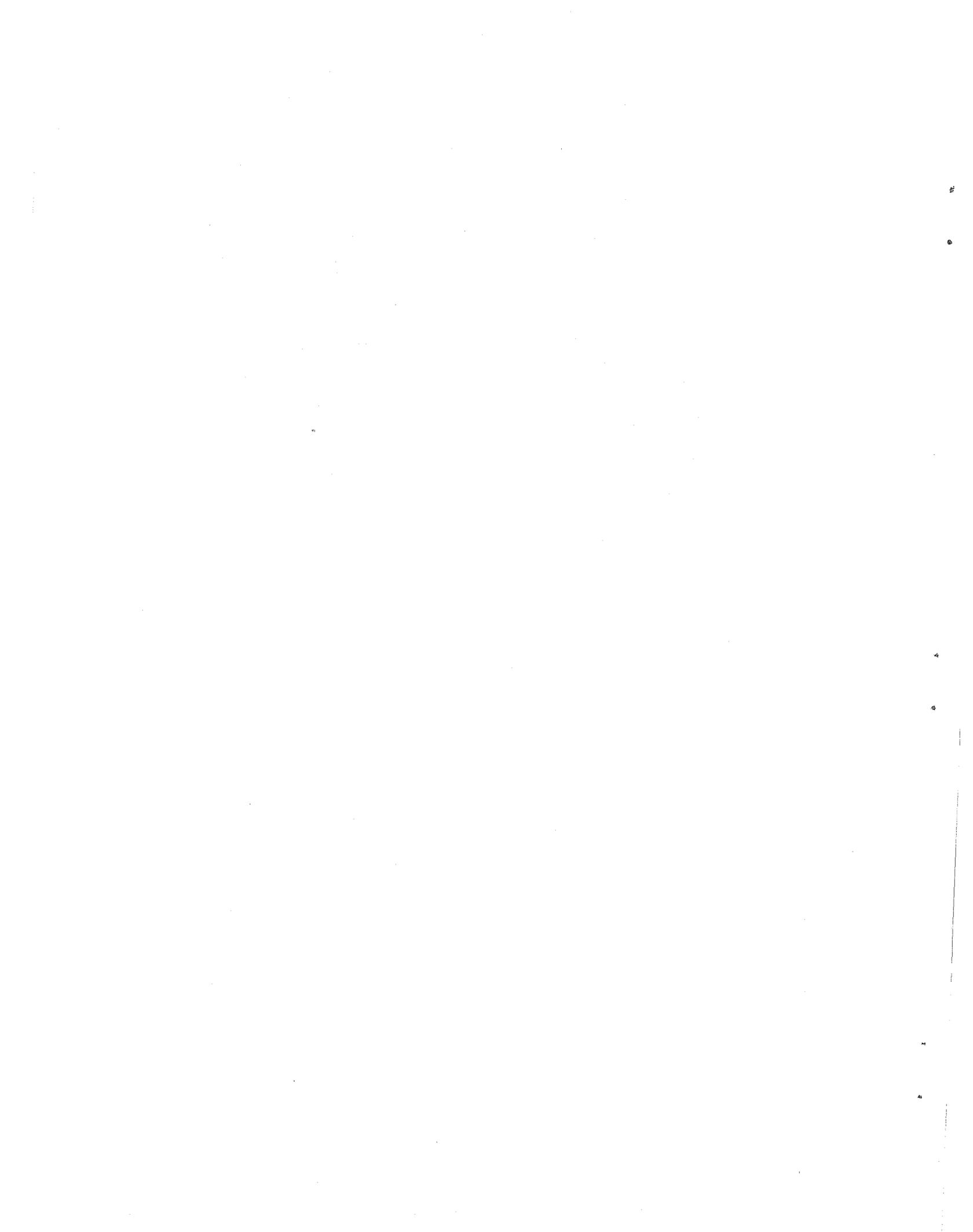


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ABSTRACT

The difference equations for representing the diffusion theory approximation to neutron transport depend on the method of formulation. A parameterized set of equations were implemented for slab geometry with mesh points located at material intersections. Such formulations as the mesh edge with four nearest neighbors on planes are included by the equations, as well as the higher coupling of eight nearest neighbors on planes for such formulations as linear finite element. The formulations of primary interest were applied to two dimensional problems, and to three dimensional problems with coupling to nearest neighbors on planes. Solutions were obtained to multigroup problems over a wide range of problem type. Selected results are reported and conclusions regarding the formulations.



I. DISCUSSION

Background

This report documents an exploration of the difference equations for approximating neutron transport with diffusion theory in slab geometry. A variety of approaches produce different formulations. A parameterized formulation coupling near neighbor meshpoints on material interfaces was implemented in the VANCER computer code treating up to three space dimensions. Results were obtained for a wide variety of problems. This testing on problems representative of application allows conclusions to be drawn about a preferred formulation.

In 1965 we elected to move the location of the mesh points from the material intersections, as used in the earlier ORNL codes such as EXTERMINATOR¹ to the centers of the elemental volumes when the programming started on the CITATION neutronics code². With mesh points located internally, the reaction rates are accurately represented, considering that the neutron flux value at the point is a reasonable approximation of the average over the elemental volume. The net leakage between points is the same as with a mesh intersection formulation inside homogeneous materials with uniform spacing. However, the approximation across material interfaces is rather crude compared to that of mesh edge (the meshpoints located on intersections), which results in no interfaces between adjacent meshpoints. Simple tests indicated that the two formulations had about the same error associated with the finite difference formulation when modest differences in the diffusion coefficient occurred between adjacent materials. Even with large differences in the diffusion coefficients, the difference in accuracy between the two methods was found to be usually small, at least small relative to the error associated with applying a finite difference formulation.

Recall that in those days, the state of the art was such that generally only two space dimensions could be treated. The computation cost of treating three dimensions could seldom be justified. However, we often needed the capability to treat three dimensions, at least

in a coarse mesh model, to assess effects not easily taken into account by treating fewer than the full three-dimensional reactor core. Also, the emphasis in the CITATION code development was to treat a reactor operating history to the point of refueling, and further, with selective and delayed recycle.

We found that the computation cost could be minimized by locating mesh points at the centers of the elemental volumes. Only one set of nuclear properties were required at each point, as to determine fission source or downscattering, rather than weighting the properties of abutting materials. Further, the implementation cost was lower (starting from scratch) due to simpler coding. A further advantage was the improvement in the results reported: each point had a single power density and other characteristics. A disadvantage came from the incomplete assessment of peaking by assessing only the conditions at mesh point locations, so that a peak power density at a material interface was not identified, and this leaves much to be desired in many applications. (However, interpolation between results at mesh point locations can not be expected to have high reliability.)

In implementing extended capability in the VENTURE code,³ effort directed at fast reactor applications, the mesh centered formulation was used. This formulation had found wide acceptance at many installations. Extended capability was made available at low computation cost, including provision for the fission source distribution function to be material dependent (accounting for the difference between core and blanket of a breeder reactor), and also the use of a simple P_1 approximation which involves carrying a net $\nabla \cdot J$ term to correct the scattering source. These extensions are not simply implemented with mesh points located on material interfaces and would add more to the cost of computation.

Why then implement the capability to locate mesh points on material interfaces? There were several reasons. Special capability is needed in analysis to treat complicated geometries. We rule out the use of a mesh centered formulation as being unreliable for treating the skewed triangles needed to describe complicated geometries simply, like the cylindrical control rod in a hexagonal assembly, or the core containing badly distorted

fuel assemblies. What formulation should be used if the points are located on vertices of triangles? Is the finite element approach superior? Thus we have attempted to produce information needed to guide continuing effort on diffusion theory methods development and implementation.

A qualification is placed on the information reported herein due to the objective of the effort. This objective was the identification of preferred formulations for treating representative reactor core problems with diffusion theory which require a three-dimensional representation.

Regarding Available Information

There is published information about the subject. Unfortunately the reader is often led to believe that a particular method, especially a new one, is superior to all others. Limited testing of different formulations and limited comparative evaluation of the different methods leave us unable to make reliable judgements and decision. Often the problems which will arise in application have not been identified, nor techniques proven to produce reliable results in wide application on a routine basis.

There is published information which indicates that the mesh centered formulation is inferior to the mesh edge formulation. Excepting certain applications, and the triangular mesh situation discussed later, we find the mesh centered formulation to be generally acceptable and often the most cost effective of the two.

Application of "higher-order" Taylor series expansion formulations has been tested at BAPL.⁴

Representative Application

In serious reactor core analysis, there are many zones of different nuclide compositions and hence macroscopic properties. Even though a first core may have large homogeneous zones (often requiring homogenization to eliminate a fine scale detail which can not be treated),

after exposure the nuclide densities and hence macroscopic properties vary continuously over the reactor. Since this variation must be taken into account, a large number of zones having different macroscopic properties must be considered. Likely a lower bound for reliable analysis is $10^3 = 1,000$ zones in three dimensions, and more may be required. Likely at least $20^3 = 8,000$ mesh points are required just to adequately account for the geometric variations, and often many more. So we start with the assumption that there are many mesh points.

The test problems normally used to evaluate methods are not representative of requirements. The clean core problems must of course be solved, but these are a small subset of those of interest. Identifying the method which produces the most accurate results, or the lowest cost of computation for a given accuracy, for simple problems, probably makes a negative contribution by a false generalization.

There is need in analysis for methods which treat simple geometric arrangements at low computation costs. If a reactor history is to be followed through several refuelings, severe compromises must be made to hold down the computation cost to even a reasonable level. The state of the art is yet such that detailed three-dimensional modeling with many neutron energy groups can seldom be done. The cost is prohibitive. Therefore, coarse modeling is usually necessary, and certainly parametric survey studies must be done without consideration of fine detail. The state of the art is such that two-dimensional analysis can be done, one-dimensional calculations must often be utilized, and special schemes are very useful. Thus the separability approximation, synthesis of some form, and other techniques are needed.

In this effort we are primarily interested in a method which admits treating considerable detail and is adequate when the geometry is simple.

The Neighbor Coupling Penalty

In slab geometry, a mesh point has four nearest neighbors on a plane and two on adjacent planes, total six. Thus in the lowest order approximation of transport, the leakage associated with an elemental volume is through the six surfaces, and the difference equation yields a dependence of the flux at a point on the values of the flux at these six neighbors. So with either the mesh center or mesh edge formulations

in wide use, a point has six neighbors, minimal coupling. Actually there are eight close neighbors to a point on a plane and nine on each of the neighboring planes, a total of twenty-six close neighbors.

Any sophisticated formulation of the flux distribution over the elemental volume about a mesh point involves coupling these twenty-six neighbors. Application of the finite element method in its lowest order, linear, results in such coupling. The incremental cost of computation due to this increase in coupling is difficult to justify. Either the error in the results must be sufficiently reduced to justify the increased cost, or it must be possible to reduce the number of mesh points in the problem to offset it.

Note that higher order formulations which couple in more than just the close neighbors, significantly increase the number of points involved, and increase the computation cost.

Methods Backup

Considerable effort went into analysis of and understanding the various difference formulations obtained from different approaches. Thus the one-dimensional equations can be displayed and tested. Explicit solutions can be obtained for one-group, bare reactor problems treating up to three dimensions. Documenting this effort is beyond the scope of this report. However, this backup effort was of crucial importance and produced information which was used to select between major options. The following comments are offered.

1. Rather complicated techniques may be used to develop the difference formulations. Thus a two-dimensional finite element scheme on planes may be used with a simple difference formulation to couple between planes. This admits sophistication across fuel assemblies without serious impact from the treatment of the third dimension. The results can have higher accuracy than obtained with the simple mesh edge difference formulation and may well be used to advantage.
2. The incremental cost of computation can not be justified to couple more than close neighbors (using higher ordered formulations), and likely is not justified to treat more than near neighbors in the axial coordinate if the method is to be competitive.

3. The relatively high accuracy of the equations resulting from the usual finite element scheme in its lowest order (linear), in spite of the weak formulation, came as a surprise; theoretical justification for this is not evident.
4. Whereas the simple difference equations admit only positive flux solutions given positive nuclear properties, indiscriminate application of other formulations admit negative solutions. Generally positive results are assured only if the mesh spacing is less than

$$\Delta < \sqrt{\frac{D}{\alpha \Sigma}} ,$$

where D is the diffusion coefficient, Σ is the removal cross section, and α is a parameter which depends on the formulation method ($\alpha = 0$ for the simple difference formulations). This is a rather severe bound. A code written for playing games can be allowed to do anything, but one for general application must address this difficulty and hopefully take action to prevent the generation of negative flux values, an acceptable mathematical solution but unacceptable in application, especially since the multiplication factor may not be simply associated with a unique and most positive eigenvalue.

5. An overall neutron balance is complicated. Some codes, at least the ones we have developed, require that an overall neutron balance be satisfied and allow the multiplication factor to be estimated from it. The usual boundary conditions can readily be satisfied (non-return, zero derivative, and even the less important zero flux) but the sum of the difference equations leaves special boundary terms which must be accounted for.
6. There are surprises in treating two and three dimensions not evident in one dimensional analysis. Not only must cross derivative terms be ignored in a Taylor expansion approach, but rather simple approximations which seem reasonable produce unacceptable solutions.
7. It is practical to introduce free parameters in the difference equations. These take on specific values for the difference equations which result from a method of development, and admit variation in the values over a wide range, useful for testing and possibly in application. Implementation of procedures to admit these free parameters is relatively easy if the equations are written out to express the dependence throughout the calculational procedure (as if we ever do this before starting a program!).

8. Examination of the dominant error vector eigenvalues on inner and outer iteration indicates that they have but small dependence on the formulation. It is of interest that fixing the number of mesh points, the outer iteration eigenvalue was found to increase as the size of a bare reactor increases (fixed nuclear properties) while the inner iteration eigenvalue decreased.
9. Results indicate that significant improvement over the simple difference formulations can not be expected if the source and removal terms are treated differently. It is attractive to reduce computation cost by using the average local source, but a better approximation of the flux distribution over an elemental volume for the removal. Although this can be done, it is highly recommended against, because it can produce inferior results in many situations.

Remark on Hexagonal Geometry

The hexagonal fuel assembly presents a special situation. With the mesh point centered in an assembly, each point has six nearest neighbors on the plane equally distant, and the leakage across the associated six surfaces should be a reasonable approximation. (In slab geometry there are four neighbors and four leakage surfaces.) With mesh centered triangular geometry, six points per hexagon, a point has only three neighbors. Leakage is treated across only three surfaces, and is a rather coarse approximation. Locating the mesh points at the triangle corners (one on each corner of the hexagon and one at the center) causes each point to have six neighbors, and the six leakage surfaces admit a reliable leakage approximation. In the lowest-order mesh centered formulation for triangles, each hexagon has six points. With one point in the center and each corner point shared by three hexagons, only three points are associated with each hexagon (although boundaries reduce sharing). So about half as many points are required as mesh centered and the leakage approximation is improved. Thus as the formulation goes from 3 to 6 points per hexagon, doubling the number of points, an expected reduction in the difference approximation error may not occur. Extensive testing has been done on problems of interest, some of which is reported in the literature,⁵ which indicates that the mesh centered formulation may not be the preferred one. More sophisticated approximation of the flux distribution has also been done with good results.⁶

Remark on the Internal Black Absorber

We have done only a small amount of testing in application of the internal black absorber representation. This approximation is useful for representing control rod explicitly in the thermal range in a thermal reactor, and for blocking out a section of the geometric description. An extrapolation distance into the absorber is used to estimate the flux derivative at the surface relative to the flux, a non-return boundary condition yielding the net leakage rate of neutrons across the surface. We do note that carrying along this formulation complicates the coding and also the accounting, as in an overall neutron balance. We have used schemes of approximating the internal leakage using both the next-to-latest iterate flux values and the latest ones to reduce the amount of calculation required to determine the multiplication factor with an overall neutron balance. The discrepancy should usually be small and not impact the iterative process except when the leakage is a large fraction of the total neutron loss rate.

We are aware of good experience in representing internal black absorbers with the mesh centered formulation. This is perhaps surprising when the value of the flux at the surface is not calculated, but on the other hand the linear approximation of the flux outside the absorber is made from the mesh point to the surface, not all the way across the adjacent differential element.

On Solving the Equations

The usual inner, outer iteration scheme was used to solve problems. Although undoubtedly there is a class of problems up to some size which can be solved economically by direct inversion of the space problem, this scheme simply is not competitive when a large amount of data must be moved in and out of computer memory.⁷ With usual iteration schemes, the data is carefully partitioned into the needed blocks to support sweeping the mesh in iteration. With only local coupling between points in space, the band width of needed data is narrow, a small amount of data is involved in comparison with the filled matrices which must be treated with direct inversion. The data handling burden can not be ignored in serious implementation effort.

II. IMPLEMENTATION

A copy of an early version of the VENTURE code was used as a starting point. Major revisions were made to the basic data handling procedures. Only the "multi-plane-stored" mode of calculation was retained, which limits application to two-dimensional problems which can be held in memory for inner iteration at each group.

The coupling interface data file specifications were modified to allow an interpretation in the sense of the mesh edge formulation.

The routines which generate the equation coefficients for slab geometry were revised to introduce the parameterized mesh edge formulations. These involve either four nearest neighbors on planes or the eight close neighbors on option, and the nearest neighbor on each adjacent plane.

The iteration routines were modified to treat the equations. The changes include treating the full coupling on option, consistent source calculation or use of the local source on option, and consistent calculation of the multiplication factor from an overall neutron balance, and from the residues approach on termination.

Average flux and power density values were generated and printed for the elemental volumes each surrounded by mesh points. This step of processing is deemed to be quite essential to support testing and for general application. The zone, group flux values were placed in the file needed for exposure calculations. Thus depletion capability with this code was made available by implementing it in parallel with the VENTURE code in the local system for core analysis.

Calculational Procedure

The basic procedure of calculation was that documented in the VENTURE code report with modest changes. A reordering of the iterative procedure was done to facilitate the estimation of the multiplication factor from the overall neutron balance because additional information was required. A number of improvements in the VENTURE code which were

incorporated prior to the version 2 release were not incorporated in VANCER. These include modifications to the acceleration procedures on both inner and outer iteration.

The Programmed Equations

The equations which were applied are presented here. A mesh point and its close neighbors are shown in Fig. 1. Also shown are the mesh dimensions considering a specific point (the mesh spacing varies), and the local material properties. Note the subset two-dimensional mesh located on a plane. Only the nearest mesh point on each adjacent plane is considered in writing the difference equations for the element associated with a mesh point in three dimensions. A leading coefficient of 2 for each coordinate has been cancelled out of the equations, 8 in three dimensions.

The point flux value is calculated in the iterative process as dependent on close neighbor values as

$$\begin{aligned} \phi(J,I,B,K) = & \\ & \left[\phi(J-1,I,B,K) * DR(J,I,B,K) + \phi(J+1,I,B,K) * DR(J+1,I,B,K) \right. \\ & + \phi(J,I-1,B,K) * DB(J,I,B,K) + \phi(J,I+1,B,K) * DB(J,I+1,B,K) \\ & + \phi(J,I,B-1,K) * DA(J,I,B,K) + \phi(J,I,B+1,K) * DA(J,I,B+1,K) \\ & + \phi(J+1,I+1,B,K) * DH(J,I,B,K) \\ & + \phi(J+1,I-1,B,K) * DH(J,I-1,B,K) \\ & + \phi(J-1,I-1,B,K) * DH(J-1,I-1,B,K) \\ & + \phi(J-1,I+1,B,K) * DH(J-1,I,B,K) \\ & \left. + TS(J,I,B) \right] / TL(J,I,B,K) . \end{aligned}$$

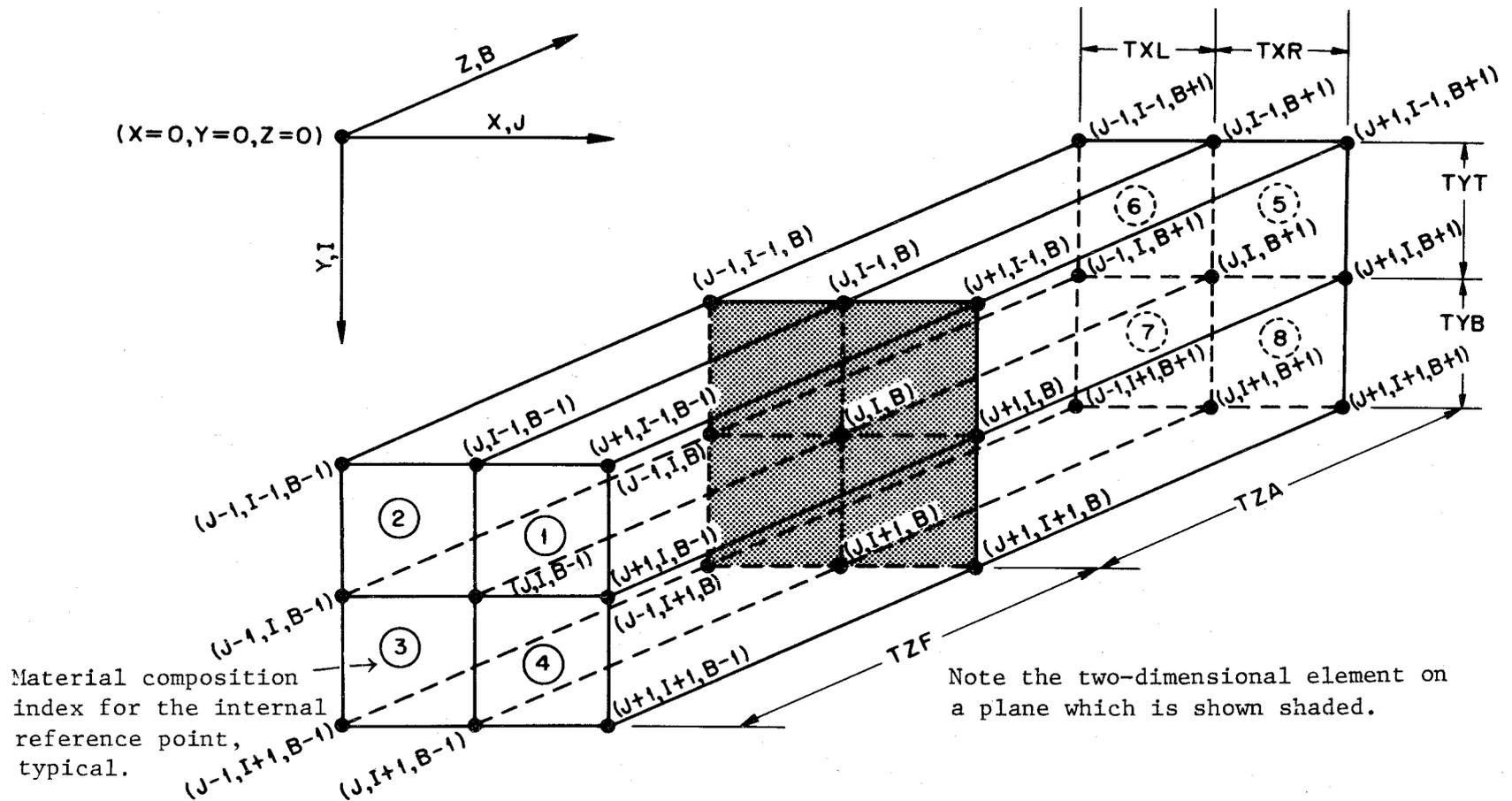


Fig. 1. The Finite Difference Element.

where:

$$\begin{aligned}
 DR(J,I,B,K) = & \\
 & \alpha_1 * \left[\frac{TYT * TZF}{TXL} * D(2,K) + \frac{TYB * TZF}{TXL} * D(3,K) \right. \\
 & \left. + \frac{TYT * TZA}{TXL} * D(6,K) + \frac{TYB * TZA}{TXL} * D(7,K) \right] \\
 & - \alpha_2 * \left[TXL * TYT * TZF * \Sigma(2,K) + TXL * TYB * TZF * \Sigma(3,K) \right. \\
 & \left. + TXL * TYT * TZA * \Sigma(6,K) + TXL * TYB * TZA * \Sigma(7,K) \right] \\
 & - \alpha_5 * \left[\frac{TXL * TZF}{TYT} * D(2,K) + \frac{TXL * TZF}{TYB} * D(3,K) \right. \\
 & \left. + \frac{TXL * TZA}{TYT} * D(6,K) + \frac{TXL * TZA}{TYB} * D(7,K) \right] , \text{ or}
 \end{aligned}$$

$$\begin{aligned}
 DR(J,I,B,K) = & \\
 & 2 * \alpha_0 * \left[TYT * TZF * C_2 + TYB * TZF * C_3 + TYT * TZA * C_6 + TYB * TZA * C_7 \right]
 \end{aligned}$$

for extrapolated or non-return boundaries.

$$\begin{aligned}
 DR(J+1,I,B,K) = & \\
 & \alpha_1 * \left[\frac{TYT * TZF}{TXR} * D(1,K) + \frac{TYB * TZF}{TXR} * D(4,K) \right. \\
 & \left. + \frac{TYT * TZA}{TXR} * D(5,K) + \frac{TYB * TZA}{TXR} * D(8,K) \right] \\
 & - \alpha_2 * \left[TXR * TYT * TZF * \Sigma(1,K) + TXR * TYB * TZF * \Sigma(4,K) \right. \\
 & \left. + TXR * TYT * TZA * \Sigma(5,K) + TXR * TYB * TZA * \Sigma(8,K) \right]
 \end{aligned}$$

$$-\alpha_5 * \left[\frac{TXR * TZF}{TYT} * D(1,K) + \frac{TXR * TZF}{TYB} * D(4,K) \right. \\ \left. + \frac{TXR * TZA}{TYT} * D(5,K) + \frac{TXR * TZA}{TYB} * D(8,K) \right], \text{ or}$$

$$DR(J+1, I, B, K) =$$

$$2 * \alpha_0 * \left[TYT * TZF * C_1 + TYB * TZF * C_4 + TYT * TZA * C_5 + TYB * TZA * C_8 \right]$$

for extrapolated or non-return boundaries.

$$DB(J, I, B, K) =$$

$$\alpha_1 * \left[\frac{TXL * TZF}{TYT} * D(2,K) + \frac{TXR * TZF}{TYT} * D(1,K) \right. \\ \left. + \frac{TXL * TZA}{TYT} * D(6,K) + \frac{TXR * TZA}{TYT} * D(5,K) \right] \\ - \alpha_2 * \left[TXL * TYT * TZF * \Sigma(2,K) + TXR * TYT * TZF * \Sigma(1,K) \right. \\ \left. + TXL * TYT * TZA * \Sigma(6,K) + TXR * TYT * TZA * \Sigma(5,K) \right]$$

$$-\alpha_5 * \left[\frac{TYT * TZF}{TXL} * D(2,K) + \frac{TYT * TZF}{TXR} * D(1,K) \right. \\ \left. + \frac{TYT * TZA}{TXL} * D(6,K) + \frac{TYT * TZA}{TXR} * D(5,K) \right], \text{ or}$$

$$DB(J, I, B, K) =$$

$$2 * \alpha_0 * \left[TXL * TZF * C_2 + TXR * TZF * C_1 + TXL * TZA * C_6 + TXR * TZA * C_5 \right]$$

for extrapolated or non-return boundaries.

$$DB(J, I+1, B, K) =$$

$$\begin{aligned} & \alpha_1 * \left[\frac{TXL * TZF}{TYB} * D(3, K) + \frac{TXR * TZF}{TYB} * D(4, K) \right. \\ & \quad \left. + \frac{TXL * TZA}{TYB} * D(7, K) + \frac{TXR * TZA}{TYB} * D(8, K) \right] \\ & - \alpha_2 * \left[TXL * TYB * TZF * \Sigma(3, K) + TXR * TYB * TZF * \Sigma(4, K) \right. \\ & \quad \left. + TXL * TYB * TZA * \Sigma(7, K) + TXR * TYB * TZA * \Sigma(8, K) \right] \\ & - \alpha_5 * \left[\frac{TYB * TZF}{TXL} * D(3, K) + \frac{TYB * TZF}{TXR} * D(4, K) \right. \\ & \quad \left. + \frac{TYB * TZA}{TXL} * D(7, K) + \frac{TYB * TZA}{TXR} * D(8, K) \right] , \text{ or} \end{aligned}$$

$$DB(J, I+1, B, K) =$$

$$2 * \alpha_0 * \left[TXL * TZF * C_3 + TXR * TZF * C_2 + TXL * TZA * C_7 + TXR * TZA * C_8 \right]$$

for extrapolated or non-return boundaries.

$$DA(J, I, B, K) =$$

$$\begin{aligned} & \alpha_8 * \left[\frac{TXL * TYT}{TZF} * D(2, K) + \frac{TXR * TYT}{TZF} * D(1, K) \right. \\ & \quad \left. + \frac{TXL * TYB}{TZF} * D(3, K) + \frac{TXR * TYB}{TZF} * D(4, K) \right] \\ & - \alpha_9 * \left[TXL * TYT * TZF * \Sigma(2, K) + TXR * TYT * TZF * \Sigma(1, K) \right. \\ & \quad \left. + TXL * TYB * TZF * \Sigma(3, K) + TXR * TYB * TZF * \Sigma(4, K) \right] , \text{ or} \end{aligned}$$

$$DA(J,I,B,K) =$$

$$2*\alpha_0 * \left[TXL * TYT * C_2 + TXR * TYT * C_1 + TXL * TYB * C_3 + TXR * TYB * C_4 \right]$$

for extrapolated or non-return boundaries.

$$DA(J,I,B+1,K) =$$

$$\begin{aligned} & \alpha_8 * \left[\frac{TXL * TYT}{TZA} * D(6,K) + \frac{TXR * TYT}{TZA} * D(5,K) \right. \\ & \quad \left. + \frac{TXL * TYB}{TZA} * D(7,K) + \frac{TXR * TYB}{TZA} * D(8,K) \right] \\ & -\alpha_9 * \left[TXL * TYT * TZA * \Sigma(6,K) + TXR * TYT * TZA * \Sigma(5,K) \right. \\ & \quad \left. + TXL * TYB * TZA * \Sigma(7,K) + TXR * TYB * TZA * \Sigma(8,K) \right], \text{ or} \end{aligned}$$

$$DA(J,I,B+1,K) =$$

$$2*\alpha_0 * \left[TXL * TYT * C_6 + TXR * TYT * C_5 + TXL * TYB * C_7 + TXR * TYB * C_8 \right]$$

for extrapolated or non-return boundaries.

$$DH(J,I,B,K) =$$

$$\begin{aligned} & \alpha_3 * \left[\left(\frac{TYB * TZF}{TXR} + \frac{TXR * TZF}{TYB} \right) * D(4,K) \right. \\ & \quad \left. + \left(\frac{TYB * TZA}{TXR} + \frac{TXR * TZA}{TYB} \right) * D(8,K) \right] \\ & -\alpha_4 * \left[TXR * TYB * TZF * \Sigma(4,K) + TXR * TYB * TZA * \Sigma(8,K) \right] \end{aligned}$$

$$DH(J-1,J,B,K) =$$

$$\begin{aligned} & \alpha_3 * \left[\left(\frac{TYB * TZF}{TXL} + \frac{TXL * TZF}{TYB} \right) * D(3,K) \right. \\ & \quad \left. + \left(\frac{TYB * TZA}{TXL} + \frac{TXL * TZA}{TYB} \right) * D(7,K) \right] \end{aligned}$$

$$-\alpha_4 * \left[\text{TXL} * \text{TYB} * \text{TZF} * \Sigma(3, \text{K}) + \text{TXL} * \text{TYB} * \text{TZA} * \Sigma(7, \text{K}) \right] .$$

$$\text{DH}(\text{J}, \text{I}-1, \text{B}, \text{K}) =$$

$$\alpha_3 * \left[\left(\frac{\text{TYT} * \text{TZF}}{\text{TXR}} + \frac{\text{TXR} * \text{TZF}}{\text{TYT}} \right) * \text{D}(1, \text{K}) \right.$$

$$\left. + \left(\frac{\text{TYT} * \text{TZA}}{\text{TXR}} + \frac{\text{TXR} * \text{TZA}}{\text{TYT}} \right) * \text{D}(5, \text{K}) \right]$$

$$-\alpha_4 * \left[\text{TXR} * \text{TYT} * \text{TZF} * \Sigma(1, \text{K}) + \text{TXR} * \text{TYT} * \text{TZA} * \Sigma(5, \text{K}) \right] .$$

$$\text{DH}(\text{J}-1, \text{I}-1, \text{B}, \text{K}) =$$

$$\alpha_3 * \left[\left(\frac{\text{TYT} * \text{TZF}}{\text{TXL}} + \frac{\text{TXL} * \text{TZF}}{\text{TYT}} \right) * \text{D}(2, \text{K}) \right.$$

$$\left. + \left(\frac{\text{TYT} * \text{TZA}}{\text{TXL}} + \frac{\text{TXL} * \text{TZA}}{\text{TYT}} \right) * \text{D}(6, \text{K}) \right]$$

$$-\alpha_4 * \left[\text{TXL} * \text{TYT} * \text{TZF} * \Sigma(2, \text{K}) + \text{TXL} * \text{TYT} * \text{TZA} * \Sigma(6, \text{K}) \right] .$$

$$\text{TS}(\text{J}, \text{I}, \text{B}) = \frac{\chi(\text{K})}{\text{k}} * \text{TFS}(\text{J}, \text{I}, \text{B}) + \text{TSS}(\text{J}, \text{I}, \text{B}) .$$

$$\text{TL}(\text{J}, \text{I}, \text{B}, \text{K}) =$$

$$\alpha_0 * \left[\text{TXL} * \text{TYT} * \text{TZF} * \Sigma(2, \text{K}) + \text{TXR} * \text{TYT} * \text{TZF} * \Sigma(1, \text{K}) \right.$$

$$+ \text{TXL} * \text{TYB} * \text{TZF} * \Sigma(3, \text{K}) + \text{TXR} * \text{TYB} * \text{TZF} * \Sigma(4, \text{K})$$

$$+ \text{TXL} * \text{TYT} * \text{TZA} * \Sigma(6, \text{K}) + \text{TXR} * \text{TYT} * \text{TZA} * \Sigma(5, \text{K})$$

$$\left. + \text{TXL} * \text{TYB} * \text{TZA} * \Sigma(7, \text{K}) + \text{TXR} * \text{TYB} * \text{TZA} * \Sigma(8, \text{K}) \right]$$

$$+ \text{DR}(\text{J}, \text{I}, \text{B}, \text{K}) + \text{DR}(\text{J}+1, \text{I}, \text{B}, \text{K}) + \text{DB}(\text{J}, \text{I}, \text{B}, \text{K}) + \text{DB}(\text{J}, \text{I}+1, \text{B}, \text{K})$$

$$+ \text{DA}(\text{J}, \text{I}, \text{B}, \text{K}) + \text{DA}(\text{J}, \text{I}, \text{B}+1, \text{K}) + \text{INTERNAL BLACK BOUNDARY LOSSES}$$

$$+ \text{DH}(\text{J}, \text{I}, \text{B}, \text{K}) + \text{DH}(\text{J}-1, \text{I}, \text{B}, \text{K}) + \text{DH}(\text{J}, \text{I}-1, \text{B}, \text{K}) + \text{DH}(\text{J}-1, \text{I}-1, \text{B}, \text{K}) .$$

$$\begin{aligned}
\text{TFS}(J, I, B) = & \\
& \left[\text{TXR} * \text{TYT} * \text{TZF} * \text{FS}(1, J, I, B) + \text{TXL} * \text{TYT} * \text{TZF} * \text{FS}(2, J, I, B) \right. \\
& + \text{TXL} * \text{TYB} * \text{TZF} * \text{FS}(3, J, I, B) + \text{TXR} * \text{TYB} * \text{TZF} * \text{FS}(4, J, I, B) \\
& + \text{TXR} * \text{TYT} * \text{TZA} * \text{FS}(5, J, I, B) + \text{TXL} * \text{TYT} * \text{TZA} * \text{FS}(6, J, I, B) \\
& \left. + \text{TXL} * \text{TYB} * \text{TZA} * \text{FS}(7, J, I, B) + \text{TXR} * \text{TYB} * \text{TZA} * \text{FS}(8, J, I, B) \right] \\
+ \alpha_6 * & \left[\text{TXL} * \text{TYT} * \text{TZF} * \text{FS}(1, J-1, I, B) + \text{TXL} * \text{TYB} * \text{TZF} * \text{FS}(4, J-1, I, B) \right. \\
& + \text{TXL} * \text{TYT} * \text{TZA} * \text{FS}(5, J-1, I, B) + \text{TXL} * \text{TYB} * \text{TZA} * \text{FS}(8, J-1, I, B) \\
& + \text{TXR} * \text{TYT} * \text{TZF} * \text{FS}(2, J+1, I, B) + \text{TXR} * \text{TYB} * \text{TZF} * \text{FS}(3, J+1, I, B) \\
& + \text{TXR} * \text{TYT} * \text{TZA} * \text{FS}(6, J+1, I, B) + \text{TXR} * \text{TYB} * \text{TZA} * \text{FS}(7, J+1, I, B) \\
& + \text{TXL} * \text{TYT} * \text{TZF} * \text{FS}(3, J, I-1, B) + \text{TXR} * \text{TYT} * \text{TZF} * \text{FS}(4, J, I-1, B) \\
& + \text{TXL} * \text{TYT} * \text{TZA} * \text{FS}(7, J, I-1, B) + \text{TXR} * \text{TYT} * \text{TZA} * \text{FS}(8, J, I-1, B) \\
& + \text{TXL} * \text{TYB} * \text{TZF} * \text{FS}(2, J, I+1, B) + \text{TXR} * \text{TYB} * \text{TZF} * \text{FS}(1, J, I+1, B) \\
& \left. + \text{TXL} * \text{TYB} * \text{TZA} * \text{FS}(6, J, I+1, B) + \text{TXR} * \text{TYB} * \text{TZA} * \text{FS}(5, J, I+1, B) \right] \\
+ \alpha_7 * & \left[\text{TXL} * \text{TYT} * \text{TZF} * \text{FS}(4, J-1, I-1, B) + \text{TXL} * \text{TYT} * \text{TZA} * \text{FS}(8, J-1, I-1, B) \right. \\
& + \text{TXR} * \text{TYT} * \text{TZF} * \text{FS}(3, J+1, I-1, B) + \text{TXR} * \text{TYT} * \text{TZA} * \text{FS}(7, J+1, I-1, B) \\
& + \text{TXL} * \text{TYB} * \text{TZF} * \text{FS}(1, J-1, I+1, B) + \text{TXL} * \text{TYB} * \text{TZA} * \text{FS}(5, J-1, I+1, B) \\
& \left. + \text{TXR} * \text{TYB} * \text{TZF} * \text{FS}(2, J+1, I+1, B) + \text{TXR} * \text{TYB} * \text{TZA} * \text{FS}(6, J+1, I+1, B) \right] \\
+ \alpha_{10} * & \left[\text{TXL} * \text{TYT} * \text{TZF} * \text{FS}(6, J, I, B-1) + \text{TXL} * \text{TYB} * \text{TZF} * \text{FS}(7, J, I, B-1) \right. \\
& + \text{TXR} * \text{TYT} * \text{TZF} * \text{FS}(5, J, I, B-1) + \text{TXR} * \text{TYB} * \text{TZF} * \text{FS}(8, J, I, B-1) \\
& + \text{TXL} * \text{TYT} * \text{TZA} * \text{FS}(2, J, I, B+1) + \text{TXL} * \text{TYB} * \text{TZA} * \text{FS}(3, J, I, B+1) \\
& \left. + \text{TXR} * \text{TYT} * \text{TZA} * \text{FS}(1, J, I, B+1) + \text{TXR} * \text{TYB} * \text{TZA} * \text{FS}(4, J, I, B+1) \right] .
\end{aligned}$$

$$FS(M,J,I,B) = \sum_{L=1}^{KMAX} v\Sigma_f(M,L) * \phi(J,I,B,L) .$$

TSS(J,I,B) = Same as TFS(J,I,B) above except that SS(M,J,I,B) replaces FS(M,J,I,B),

where

$$SS(M,J,I,B) = \sum_{L=1}^{KMAX} \Sigma_s(M,L) * \phi(J,I,B,L) .$$

Where:

ϕ = neutron flux.

D = diffusion coefficient.

C = effective leakage constant for extrapolated or non-return boundaries.

Σ = total removal cross section including absorption, buckling, and outscatter.

χ = fission spectrum

k = multiplication factor.

$v\Sigma_f$ = fission production cross section.

Σ_s = inscatter cross section.

J,I,B = mesh point location index, x,y,z, where z is across planes.

K = energy group index.

KMAX = number of energy groups.

M = zone index.

The parameter coefficients α are discussed next.

Values of the Parameters

A set of input parameters is converted to the α values used in the formulation given above. We show here the values of these input or initialization values and then the conversion. The conversion is done to cause the primary term of the source to have no multiplying parameter (rather than the primary loss term) which somewhat simplifies the calculation during iteration. These input, reference parameters assume the primary loss term has a unity leading parameter (no adjustment).

The usual difference equation used in EXTERMINATOR and many other codes has a consistent source formulation: loss and source are calculated from the local point flux values. For this usual difference formulation, an all positive solution is assured and a unique, most positive, positive eigenvalue (multiplication factor) of a problem given full coupling and all positive macroscopic cross sections. The parameters take on the following values with $a_2 = a_3 = a_4 = a_5 = b_1 = b_2 = b_3 = 0$,

Dimensions	1	2	3
Neighbors	2	4	6
a_1	2	2	2
a_6	0	0	2

Use of the local source with any set of parameters (not recommended) is effected by setting $b_1 = b_2 = b_3 = 0$.

Any set of values for the parameters can be supplied, but only a limited set can be considered to be consistent. For a consistent source, $b_1 = a_2$, $b_2 = a_4$, $b_3 = a_7$

Reference sets of parameter values were made available on a user input option. The values are shown in Table 1. The identifications assigned to the parameter sets are self explanatory. Taylor series results are obtained ignoring cross terms, and higher order obtained by relating the flux and the second derivative. Linear finite element

TABLE 1. REFERENCE SETS OF PARAMETER VALUES

Reference Formulation	Linear Finite Difference	Extended Taylor Series (High Order)	Linear Finite Element	Extended Simple Taylor Series	Usual Finite Difference	Full Compromise	Simple Compromise	Compensated Difference
<u>One-Dimensional</u>								
a_1	2	2	2	2	2	2	2	2
a_2	1/4	1/6	1/3	0	0	1/12	1/12	1/4
<u>Two, Three Dimensional</u>								
Near Neighbors (2D)	8	8	8	4	4	8	4	4
Near Neighbors (3D)	10	10	10	6	6	10	6	6
a_1	3/2	5/3	4/3	5/3	2	5/3	2	2
a_2	3/16	1/9	2/9	0	0	1/9	1/12	1/4
a_3	1/2	1/3	2/3	1/3	↓	1/3	0	0
a_4	1/16	1/36	1/9	0		1/18	0	0
a_5	1/2	1/3	2/3	1/3		1/3	0	0
a_6	2	2	2	2	2	2	2	2
a_7	1/4	1/6	1/6	0	0	1/12	1/12	1/4

parameters follow directly from minimizing the usual functional. Certain compromises were selected which appeared attractive to test.

Given the initial values of the input parameters discussed above, the calculation of values of the equation parameters was done as follows:

$$X = \begin{cases} 1.0 + b_1 \\ +b_1 + b_2 & \text{if } >1 \text{ dimension} \\ +b_3 & \text{if } 3 \text{ dimensional,} \end{cases}$$

$$F = \frac{1}{X},$$

$$\alpha_0 = F$$

$$\alpha_1 = Fa_1$$

$$\alpha_2 = Fa_2$$

$$\alpha_3 = Fa_3$$

$$\alpha_4 = Fa_4$$

$$\alpha_5 = Fa_5$$

$$\alpha_6 = Fb_1$$

$$\alpha_7 = Fb_2$$

$$\alpha_8 = Fa_6$$

$$\alpha_9 = Fa_7$$

$$\alpha_{10} = Fb_3$$

But parameters which would not be used (as when two dimensions are treated) were set 0.

Consistency

A set of values of the parameters may not be consistent with any method of derivation. One reason for implementing a number of reference sets was to insure that these are consistent. However, in this effort we desired latitude in use of possible values which may prove impractical for a code to be used in general application. We do note that if we calculate

$$X = \begin{cases} 1 - b_1 & \\ -b_1 & -b_2 \\ -b_3 & \end{cases} \begin{array}{l} \text{if } > 1 \text{ dimension} \\ \text{if } 3 \text{ dimensional,} \end{array}$$

then X must be > 0 .

We also note that positive flux values are assured only if the coupling coefficients DR, DB, DA and DH are all > 0 , although this is a severe bound.

With the above formulas, a factor of 2 has been eliminated from all of the terms for each coordinate. A direct calculation of power level yields P^* . This must be corrected by dividing by $2^n \alpha_o$, where n is the number of coordinates,

$$P^1 = \frac{P^*}{2^n \alpha_o}$$

To effect a desired power level P_o , the flux values must be multiplied by

$$X = \frac{P_o}{P^1},$$

$$X = 2^n \alpha_o \frac{P_o}{P^*}.$$

To adjust such quantities as leakage calculated with the original flux, care must be taken to properly account for both the normalization and the absence of the coefficient 2 for each coordinate.

Average Flux Values

We found it desirable to calculate average flux values in each different zone (composition). For all formulations over the differential volume defined by a set of closest neighbors, there is only one material and set of macroscopic properties. The average flux over this volume is the linear average of the flux values at the mesh points. This average was used to calculate reaction rates and such other information as power density. However, peak flux values must occur at mesh points with the formulation applied, so peak quantities were also determined for the materials abutting each mesh point.

III. RESULTS OF APPLICATION TESTING

Here we report a selected set of results obtained by application to a variety of problems. Some of these problems are simple ones described in the literature. Others have complicated geometric descriptions or cross section data, or both, and documentation of such data is beyond the scope of this report. Some of these results have been reported.

For comparison, results for the problems were obtained with the VENTURE code which contains the mesh point centered formulation.

Reliability Testing

Proofing of the programming was done by demonstrating that the same results were produced for a problem as are generated by the EXTERMINATOR-II code when the same formulation was applied. Further it was demonstrated to our satisfaction that increasing the number of mesh points with any of the formulations moved the solution toward the continuum result very nearly common to all the formulations. Often more mesh points were used for this proofing than desirable from a cost viewpoint, to avoid serious contamination by high order contributions. Quite generally given a fixed group structure and sufficient mesh points, the errors in integral quantities and local properties are nearly proportional to the square of the mesh spacing.

Reference Test Problems

The five problems selected are described below:

Problem	Description
1	Two-dimensional LWR Problem (IAEA Benchmark Problem)
2	Three-dimensional LWR Problem (IAEA Benchmark Problem)
3	Neutron Transport in a BWR Rod Bundle (Two-Dimensional 7 x 7 Fuel Assembly)
4	Highly Non-separable MIT Two-Dimensional LW Reactor Problem
5	Two-Dimensional Fast Breeder Reactor Problem

Descriptions of problems 1-3 are available in Ref. 5 (ANL-7416), as are additional detailed results and results obtained with other methods. Key results for the first problem are shown in Table 2, and the dependence of the error in the multiplication factor on the number of mesh points for the usual formulations is shown in Fig. 2. Note that extrapolated results were always obtained by assuming that the error is proportional to the mesh spacing squared, using the results for the cases having the largest and the next to the largest number of mesh points.

Key results for problem 2 are shown in Table 3, and the dependence of the error in the multiplication factor for several methods is shown in Fig. 3 (data taken from the literature).

Key results for the LWR rod bundle problem 3 are shown in Table 4. We note that the difference error is very nearly the same for the usual mesh centered and mesh edge formulations when account is taken of the number of mesh points used (there is less difference on a basis of mesh point spacing than it would seem from the raw data).

Problem 4 has been described in the literature.⁸ Key results are shown for this problem in Table 5. Also shown are results obtained at ORNL with a second order finite element formulation.⁹

TABLE 2. TWO-DIMENSIONAL, TWO-GROUP IAEA BENCHMARK PROBLEM RESULTS

Formulation (Near Neighbors)	Mesh Intervals	k_{eff}	Peak Relative Power Density	
			Internal	Near Reflector
Mesh Point Centered, VENTURE (4)	9 ²	1.03208	1.549	
	17 ²	1.02965	1.649	
	34 ²	1.02924	1.599	
	68 ²	1.02944	1.544	
	136 ²	1.02954	1.522	
	272 ²	1.02958	1.515	
Extrapolated	(∞)	1.02959	1.513	
Mesh Edge, VANCER				
Usual Finite-Difference (4)	9 ²	1.07647	none	4.28
	17 ²	1.03733	0.962	2.231
	34 ²	1.03077	1.364	1.660
	68 ²	1.02983	1.475	1.546
	(∞)	1.02952	1.512	1.508
Taylor Series (8)	34 ²	1.03080	1.364	1.652
High Order Taylor Series (8)	17 ²	1.03442	1.095	2.043
	34 ²	1.03036	1.405	1.629
	68 ²	1.02975	1.485	1.544
	(∞)	1.02955	1.512	1.516
Linear Finite-Element (8)*	17 ²	1.03109	1.309	1.779
	34 ²	1.02985	1.462	1.605
	68 ²	1.02965	1.499	1.545
	(∞)	1.02958	1.511	1.525
Linear Finite-Difference (8)*	17 ²	1.03236	1.214	1.887
	34 ²	1.03006	1.437	1.614
	68 ²	1.02969	1.493	1.544
	(∞)	1.02957	1.512	1.521
Compromise (8)	17 ²	1.03390	1.123	2.009
	34 ²	1.03028	1.412	1.625
	68 ²	1.02973	1.487	1.544
Simple Compromise (4)	(∞)	1.02955	1.512	1.517
	34 ²	1.03051	1.389	1.645
	68 ²	1.02978	1.481	1.544
Compensated Difference (4)*	(∞)	1.02954	1.512	1.510
	17 ²	1.03206	1.228	1.900
	34 ²	1.03002	1.438	1.628
	68 ²	1.02968	1.493	1.547
	(∞)	1.02957	1.511	1.520
Local Source				
H-0 Taylor Series (8)	34 ²	1.03162	1.393	1.724
Linear Finite-Element (8)	34 ²	1.03229	1.402	1.792
Linear Finite-Difference (8)	34 ²	1.03280	1.422	1.860
Compromise (8)	34 ²	1.03178	1.387	1.737
Simple Compromise (4)	34 ²	1.03126	1.375	1.700
Compensated Difference (4)	34 ²	1.03224	1.403	1.799
Apparent Solution		1.02958	1.51	1.52

* Results for 9² mesh inadequate, resulting flux skewed; the only clue of inadequate solution is a neutron balance k.

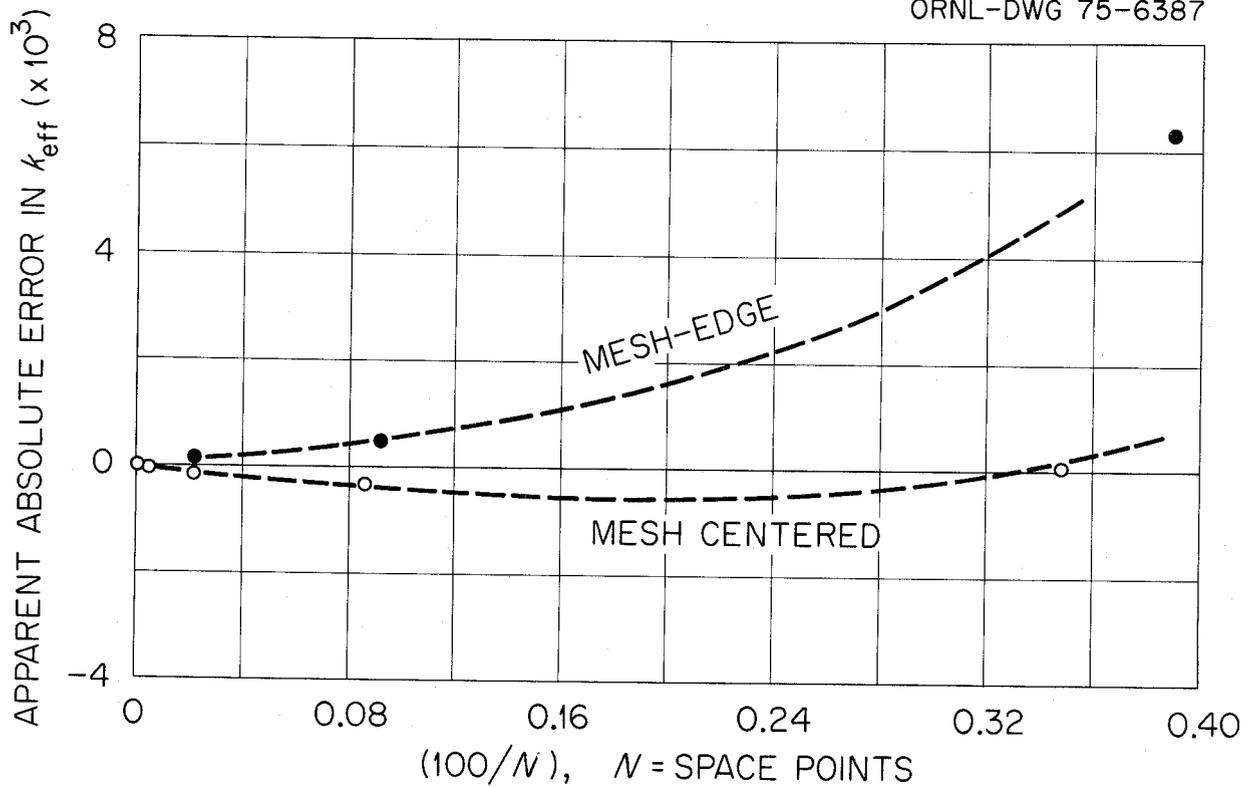


FIG. 2. TWO-DIMENSIONAL FINITE-DIFFERENCE RESULTS.

TABLE 3. THREE-DIMENSIONAL TWO-GROUP IAEA BENCHMARK PROBLEM RESULTS
(34 x 34 x 38 Mesh Points)

Formulation (Near Neighbors)	k_{eff}	Peak Power Density	
		Internal	Reflector Edge
VENTURE, Mesh Centered (6)	1.02864	2.50	2.42
Extrapolated (∞)	1.02903	2.35	
VANCER:			
Usual Finite-Difference (6)	1.03064	2.02	2.50
Linear Finite-Element (10)	1.02949	2.21	2.53
Linear Finite-Difference (10)	1.02968	2.18	2.54

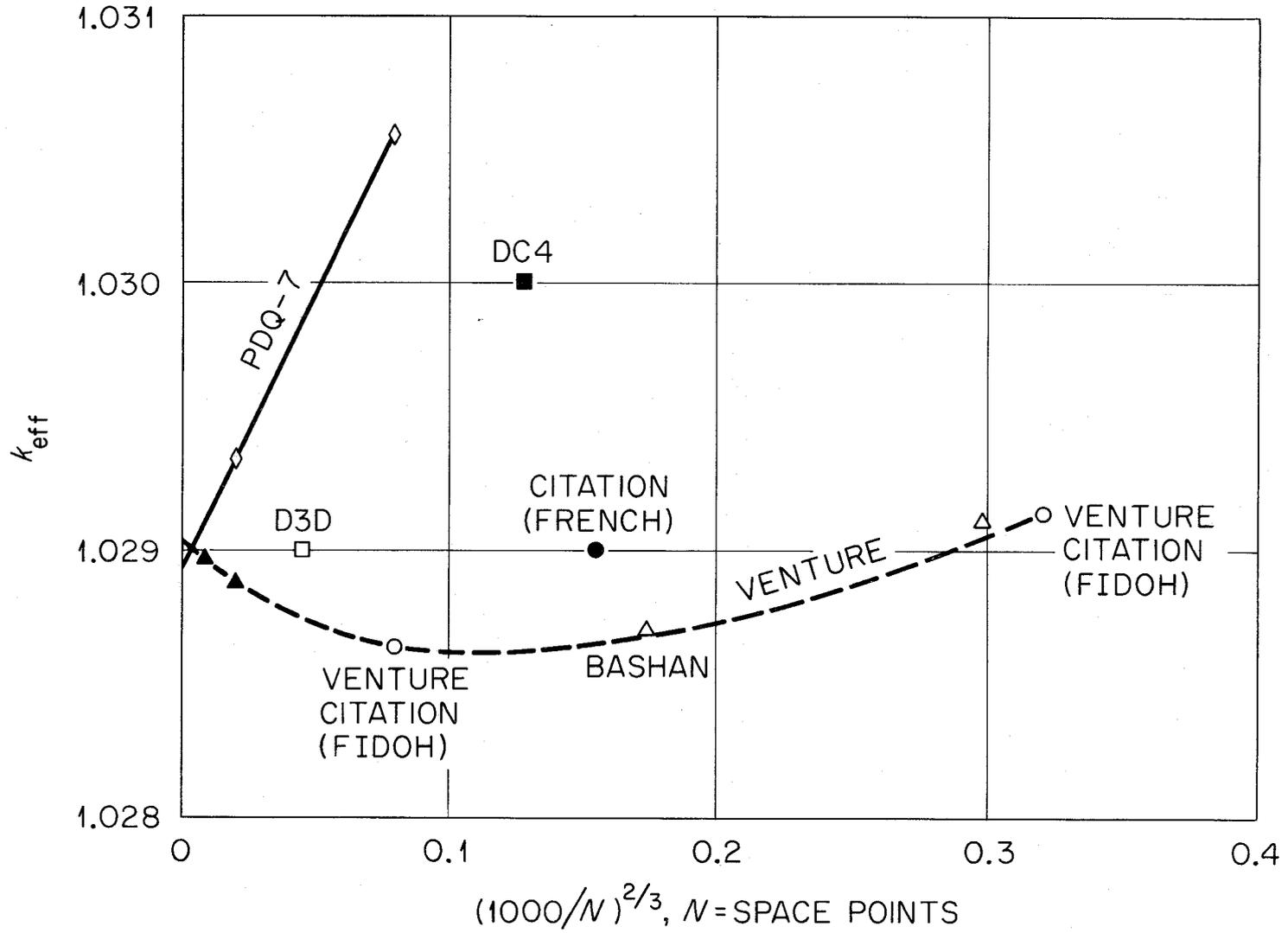


FIG. 3. THREE-DIMENSIONAL FINITE-DIFFERENCE RESULTS.

TABLE 4. LWR BUNDLE PROBLEM DIFFUSION THEORY SOLUTIONS

Mesh Points	Points Per Assembly	k_{eff}	Peak to Average Point Source	Peak Point Fast Flux	Processor Time* (min)
<u>Mesh-centered finite-difference (VENTURE)</u>					
12 x 12	1	1.09238	1.2543	0.1900	0.074
24 x 24	4	1.08759	1.3379	0.1907	0.102
48 x 48	16	1.08606	1.3851	0.1909	0.229
96 x 96	64	1.08565	1.4100	0.1910	0.921
Extrapolated	(∞)	1.0855	1.418	0.1910	
<u>Mesh-edge finite-difference (VANCER) usual finite-difference (4 neighbors)</u>					
13 x 13	(1)	1.08061	1.2607	0.1917	0.224
25 x 25	(4)	1.08389	1.3411	0.1912	0.477
49 x 49	(16)	1.08506	1.3861	0.1911	1.198
<u>Linear finite-element (8 neighbors) (VANCER)</u>					
13 x 13	(1)	1.08185	1.2659	0.1919	0.238
25 x 25	(4)	1.08454	1.3429	0.1913	0.500
49 x 49	(16)	1.08525	1.3869	0.1911	1.465

* Eigenvalue problem set up and solution; for the VENTURE solutions, the flux solution from the next smaller problem was used as a starting guess.

TABLE 5. HIGHLY NON-SEPARABLE MIT TWO-DIMENSIONAL
PROBLEM RESULTS

Formulation, Code (near neighbors)	Mesh Intervals	k_{eff}	Extrapolated k_{eff}
Mesh Centered, VENTURE (4)	23 ²	1.04275	
	31 ²	1.04188 ^a	
	40 ²	1.04408 ^b	
	62 ²	1.04033 ^a	1.0399
	124 ²	1.03990 ^a	1.03976
Quadratic Finite-Element ⁹ (18)	337	1.0391	
Mesh Edge, VANCER Usual Finite-Difference (4)	23 ²	1.03631	
	31 ²	1.03740	
	40 ²	1.03473	
	62 ²	1.03905	1.0396
Extended Taylor Series (8)	31 ²	1.03779	
Extended Higher Order Taylor Series (8)	31 ²	1.03817	
Linear Finite-Element (8)	23 ²	1.03923	
	31 ²	1.03917	
	40 ²	1.03790	
	62 ²	1.03960	1.0397
	124 ²	1.03966	1.03974
Linear Finite-Difference (8)	23 ²	1.03859	
	31 ²	1.03869	
	40 ²	1.03703	
	62 ²	1.03943	1.0397
Linear F-D, Local Source (8)	31 ²	1.04272	
Compromise (8)	23 ²	1.03786	
	31 ²	1.03823	
	40 ²	1.03621	
	62 ²	1.03930	1.0396
Compromise, Local Source (8)	31 ²	1.04087	
Compromise (4)	31 ²	1.03762	
	40 ²	1.03529	
Compromise, Local Source (4)	31 ²	1.03892	
	40 ²	1.03557	

^aConsistent mesh point expansion allowing extrapolation.

^bMesh points added to reflector traverses, a more uniform mesh spacing.

The fast breeder reactor problem 5 is rather complicated with microscopic cross sections which we do not document here due to the amount of data involved. Key results for this problem are shown in Tables 6 and 7.

Computation time was found to vary considerably. A special difficulty was the use of rather obsolete procedures in the VANCER code. We believe that the number of iterations required to solve the problems is nearly independent of the difference formulations implemented. Relative computation requirements are estimated for three-dimensional problems as follows:

<u>Formulation</u>	<u>Memory (Words)</u>	<u>Relative Computation Cost</u>
Mesh Centered (VENTURE)	166,000	1.00
Mesh Edge (VANCER)		
Six Neighbors, Consistent Source	191,000	1.37
Ten Neighbors, Consistent Source	217,000	1.73

We now make an assessment of the results for the various formulations. If one considers the difference error in the result, the number of mesh points required for each formulation can be estimated to produce the same accuracy. Then given relative cost per mesh point, the relative merit may be obtained. Thus a figure of merit may be assigned to accuracy and to cost, and the product is the relative merit of the formulation. From a practical stand-point, we may assign a higher importance to the cost because the accuracy is often adequate given the required number of points to describe the problem. We disadvantage the mesh centered formulation because its ability to show local peaking of power density (which often occurs at material interfaces) is inferior.

TABLE 6. TWO-DIMENSIONAL FAST BREEDER REACTOR PROBLEM RESULTS
(Six Neutron Groups, Slab Geometry)

<u>Formulation (Near Neighbors)</u>	<u>Mesh Intervals</u>	<u>k_{eff}</u>	<u>Peak Group 6 Flux</u>	<u>Peak Relative Power Density</u>
Mesh Centered, VENTURE (4) ^a	48 x 22	0.940161	1.089	1.9144
	96 x 44	0.938820	1.074	1.9236
Extrapolated		0.93837	1.069	1.927
Usual Finite-Difference (4)	48 x 22	0.937160	1.044	1.9351
	96 x 44	0.938055	1.061	1.9341
Extrapolated		0.93835	1.067	1.934
Linear Finite-Difference (8)	48 x 22	0.937492	1.057	1.9354
	96 x 44	0.938147	1.065	1.9345
Extrapolated		0.93837	1.068	1.934
Linear Finite-Element (8) ^b	48 x 22	0.937608	1.062	1.9358
	96 x 44	0.938176	1.066	1.9334
Extrapolated		0.93837	1.067	1.933
A Compromise (4)	48 x 22	0.937172	1.046	1.9354
A Compromise (8)	48 x 22	0.937379	1.052	1.9353
	96 x 44	0.938114	1.063	1.9331
Extrapolated		0.93836	1.067	1.932
Compensated Difference (4)	48 x 22	0.937194	1.049	1.9364
	96 x 44	0.938058	1.062	1.9335
Extrapolated		0.93835	1.066	1.932
Linear Finite-Element, Local Source (8)	48 x 22	0.942793	1.070	1.9492
Compensated Difference, Local Source (4)	48 x 22	0.941042	1.055	1.9466
Apparent Solution		0.93836	1.067	1.933

^aPeak values are inside an interval with mesh-centered points, otherwise on the edge.

^bInterval peak relative power density values: 1.8972, 1.9202, and extrapolated 1.928.

TABLE 7. PEAK POWER DENSITY FOR FAST BREEDER REACTOR PROBLEM^a

Formulation (Near Neighbors)	Mesh Intervals				
	31 ²	40 ²	62 ²	124 ²	Extrapolated
Consistent Source					
Meshpoint Centered(4) ^b	2.416	2.360	2.643	2.780	2.825
Usual Finite-Difference(4)	2.744	2.824	2.880		2.925
Taylor Series(8)	2.756				
Higher-Order Taylor Series(8)	2.803				
Linear Finite-Element(8)	2.888	2.924	2.920		2.931
Linear Finite-Difference(8)	2.850	2.898	2.910	2.927	2.933
Compromise(8)	2.813	2.873	2.900		2.928
Compromise(4)	2.772	2.842			
Compensated Difference(4)	2.831	2.878			
Local Source					
Higher-Order Taylor Series(8)	2.771				
Linear Finite-Element(8)	2.805				
Linear Finite-Difference(8)	2.789				
Compromise(8)	2.774	2.880			
Compromise(4)	2.753	2.846			
Compensated Difference(4)	2.772	2.890			

^aThe apparent result is 2.93; the reported result for the 337 point quadratic finite-element case is 2.908.

^bMesh point centered away from peak at the interface.

Shown below is the assessment:

Formulation (Near Neighbors on Planes)	Relative Merit			
	Accuracy	Cost	Accuracy x Cost	Accuracy x Cost ²
Linear Finite-Element (8)	2.8	0.8	2.2	1.8
Linear Finite-Difference (8)	2.3	0.8	1.8	1.5
Compensated Difference (4)	1.8	0.9	1.6	1.5
Compromise (8)	1.6	0.8	1.3	1.0
Mesh Centered (4)	0.9	1.4	1.3	1.8
Compromise (4)	1.2	0.9	1.1	1.0
Usual Finite Difference (4)	1.0	1.0	1.0	1.0
Local Source, Typical	0.8	1.0	0.8	0.8

Choice of the weighting of the individual values of relative merit is subject to practical considerations. For example, if the number of points required to describe the geometric arrangement is enough for the mesh centered formulation to produce a solution which is adequate for the particular calculation, then this formulation would be chosen based on cost alone. The best choice for a very coarse mesh probably would be mesh centered.

We note the low merit of the usual mesh edge formulation, and the relatively high merit of the linear finite element formulation. We caution the reader that the "higher order" formulations can be used only carefully because the use of a coarse mesh spacing will produce inadequate results. Special action should be taken in a code used routinely. The merit estimated for the mesh centered formulation reassures us in the continuing routine application of this formulation in the VENTURE and other codes.

Conclusions

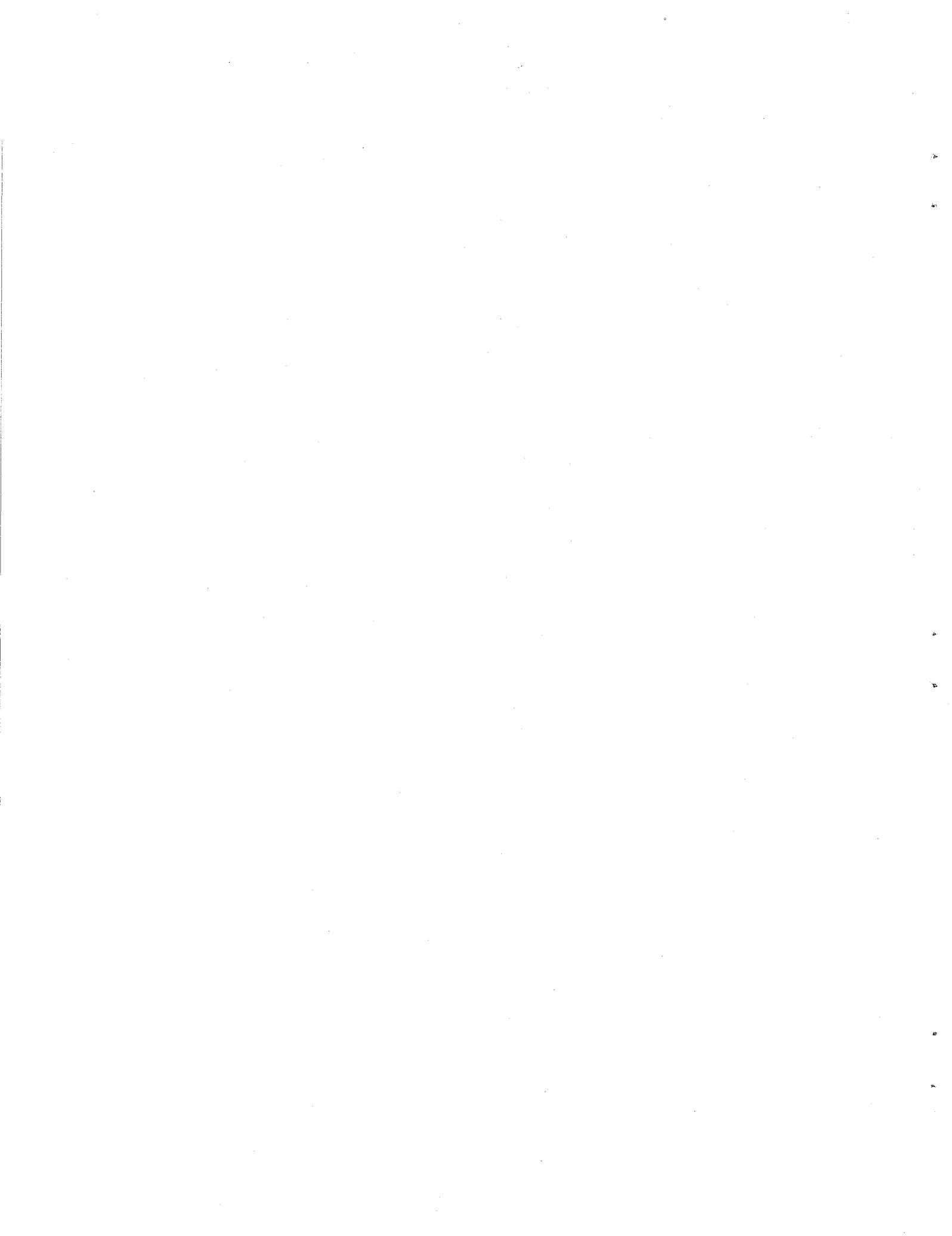
The following conclusions are drawn from this study:

1. Often the finite difference error is considerably larger than the improvement obtained by using one formulation instead of another. The common practice of using any finite difference solution as a reference result for testing methods is technically unsound, nearly as bad as using an unconverged solution.

2. Although not true in some situations, application to many problems representative of serious analysis of reflected or blanketed reactors, shows that the errors in the multiplication factor and in other properties often have opposite signs for the simple mesh edge and mesh centered formulations. The two solutions can not be considered to be bounds, because for bare reactor and cell problems, they have the same sign. Yet one would expect that a combination of the two formulations, were it practical, would generally be an improvement.
3. In most applications it appears practical to use an improved formulation on planes normal to the fuel assemblies (mesh edge), and to locate these planes of mesh points between material interfaces (mesh centered axially). Thus each point would have variation in the surrounding material on the plane, but not axially, which reduces the number of nuclear properties neighboring a point by a factor of two, reducing computation cost. The added cost of higher coupling than of just close neighbors on planes and nearest neighbors on adjacent planes can not likely be justified by the increase in accuracy.
4. The source and removal terms should be consistent; if a linear variation of the flux is assumed for calculation of removal along a coordinate, so should a linear variation of the source, which adds computation cost. We are in basic disagreement with investigators who take the opposite position on this point.
5. We find the highest accuracy from the difference equations obtained by the weak linear finite element approach provided the equations do not break down (and produce negative flux values), not well understood from a theoretical basis; this method is a form of importance weighting, considering that given the source, the space problem is self adjoint.
6. An automated procedure should be used to rectify the situation when a problem causes the implemented difference equations to break down, disallowing the admitting negative flux results, which should not be tolerated in casual application for serious analysis.
7. We have renewed confidence in the mesh centered formulation for general application because it is cost effective.
8. Location of the mesh points at corners of triangles is recommended for general triangular geometry and for treating hexagonal geometry.

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