

A NODAL METHOD FOR THREE-DIMENSIONAL
FAST-REACTOR CALCULATIONS IN HEXAGONAL GEOMETRY*

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A nodal method is developed for the solution of the multigroup neutron-diffusion equation in three-dimensional hexagonal-z geometry. The method employs an extension to hexagonal geometry of the transverse-integration procedure used extensively in the development of nodal schemes in Cartesian geometry. The partially-integrated fluxes in the three hex-plane directions are approximated by a polynomial tailored to the unique properties of the transverse-integrated equations in hexagonal geometry. The final equations, which are cast in the form of local inhomogeneous response matrix equations for each energy group, involve spatial moments of the node-interior flux distribution plus surface-averaged partial currents across the faces of the node.

Numerical calculations for models of heterogeneous-core LMFBR designs have shown the accuracy of the nodal scheme to be superior to that of the mesh-centered finite difference method using six triangular mesh cells per hexagonal fuel assembly. Particular improvement is seen in the average fluxes in the internal blanket regions and in the computed values for k-effective, thus leading to more accurate predictions of internal blanket burnups, breeding ratios, and burnup reactivity swings. This enhanced accuracy is obtained with a potential order-of-magnitude reduction in the computational cost of a three-dimensional calculation.

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*Work supported by the U. S. Department of Energy.

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INTRODUCTION

The physics and safety analysis of current Liquid Metal Fast Breeder Reactor (LMFBR) designs requires the capability to compute accurate numerical solutions in the neutron diffusion equation in three-dimensional hexagonal-z geometry. These neutronics calculations are generally performed within the U.S. fast reactor program using either standard mesh-centered finite difference codes¹ or flux synthesis methods such as the single-channel flux synthesis code SYN3D (Ref. 2). Due to the large number of unknowns involved, these calculations can be very expensive, particularly for fuel management studies which require repeated solution of the diffusion equation.

At Argonne National Laboratory, depletion calculations using the burnup code REBUS-3 (Ref. 3) are performed routinely in support of ongoing fast reactor design and analysis activities. The depletion calculation in REBUS-3 requires average group fluxes for burnup zones (over which the cross sections are taken to be spatially constant) defined such that each zone is composed of at least one hexagonal fuel assembly with an axial zone dimension of approximately 15 cm. A standard finite difference neutronics calculation requires six triangular mesh cells per hexagonal fuel assembly and an axial mesh spacing of approximately 5 cm in order to reduce spatial truncation errors to an acceptable level. Since only the zone-averaged fluxes are required for the actual depletion calculation, it is clear that a significant reduction in the overall computational expense can be achieved by reducing the number of mesh-points used to approximate the flux in each burnup zone. Thus there exists a strong motivation to develop a diffusion-theory method which will compute accurate fluxes and eigenvalues when applied on a mesh defined by the dimensions of the hexagonal fuel assemblies and the axial zone boundaries.

Nodal methods comprise a class of coarse-mesh numerical methods which have demonstrated considerable potential for the analysis of light water reactors in Cartesian geometry. Many of the earlier nodal schemes⁴ involved empirical coupling parameters which were determined from the results of detailed fine-mesh calculations or from actual operating data. Nodal schemes⁵ developed in the past eight years have, for the most part, eliminated the need for empirical constants by computing the inter-node coupling relationships using higher-order approximations to the diffusion equation. Thus, unlike the earlier ad-hoc methods, these more recent nodal schemes can be viewed as coarse-mesh approximations to the neutron diffusion equation, and can thus be expected to converge to the exact solution of the diffusion equation in the limit as the mesh spacing goes to zero.

The success of these Cartesian-geometry schemes has prompted the more recent development of analogous techniques⁶⁻⁹ for fast reactor calculations in hexagonal geometry. The nodal method⁸⁻⁹ described in this paper is based on a response matrix formulation in which the principal unknowns are surface-averaged partial currents across the nodal interfaces and spatial moments of the node-interior flux distribution. The response matrix equations are derived using an extension to hexagonal geometry of the transverse integration procedure⁵ widely used in the development of Cartesian-geometry nodal schemes. Since these equations are written separately for each energy group, application of the method to multigroup calculations is straightforward.

DERIVATION OF THE NODAL EQUATIONS

THE NODAL BALANCE EQUATION

The starting point in the derivation of the nodal scheme is the nodal balance equation obtained by integrating the multigroup neutron diffusion equation over a homogeneous hexagonal- z node. Using the orientation shown in Figure 1, with the origin (in local coordinates) taken as the center of the node, the k -th node is defined by

$$V^k: (x,y,z) \quad x \in [-h/2, +h/2], \quad y \in [-y_s(x), +y_s(x)], \quad z \in [-\Delta z^k/2, +\Delta z^k/2],$$

where

$$y_s(x) \equiv \frac{1}{\sqrt{3}} (h - |x|), \quad (1)$$

h is the lattice pitch, and Δz^k is the axial mesh spacing. Integrating the diffusion equation over the k -th node and then dividing by the node volume V^k yields the nodal balance equation

$$\frac{2}{3h} [\bar{L}_{gx}^k + \bar{L}_{gu}^k + \bar{L}_{gv}^k] + \frac{1}{\Delta z^k} \bar{L}_{gz}^k + \Sigma_g^{r,k} \bar{\phi}_g^k = \bar{Q}_g^k, \quad (2)$$

where $\bar{\phi}_g^k$ is the node-averaged flux,

$$\bar{\phi}_g^k \equiv \frac{1}{V^k} \int_{-\Delta z^k/2}^{\Delta z^k/2} dz \int_{-h/2}^{h/2} dx \int_{-y_s(x)}^{y_s(x)} dy \phi_g^k(x,y,z), \quad (3)$$

and \bar{Q}_g^k is the node-averaged multigroup source term due to fission and in-scatter into group g . The remaining terms in Eq. (2) are leakages in the three hex-plane directions and in the axial direction, e.g.

$$\bar{L}_{gx}^k \equiv \bar{J}_{gx}^k(+h/2) - \bar{J}_{gx}^k(-h/2) \quad (4)$$

$$\bar{L}_{gz}^k \equiv \bar{J}_{gz}^k(+\Delta z^k/2) - \bar{J}_{gz}^k(-\Delta z^k/2), \quad (5)$$

where $\bar{J}_{gx}^k(\pm h/2)$ and $\bar{J}_{gz}^k(\pm \Delta z^k/2)$ are surface-normal components of the net current averaged over the x- and z-directed faces:

$$\bar{J}_{gx}^k(\pm h/2) \equiv \left[\frac{1}{\Delta z^k} \int_{-\Delta z^k/2}^{\Delta z^k/2} dz \frac{1}{2y_s(x)} \int_{-y_s(x)}^{y_s(x)} dy -D_g^k \frac{\partial}{\partial x} \phi_g^k(x,y,z) \right]_{x=\pm h/2} \quad (6)$$

$$\bar{J}_{gz}^k(\pm \Delta z^k/2) \equiv \frac{\Delta z^k}{V^k} \int_{-h/2}^{h/2} dx \int_{-y_s(x)}^{y_s(x)} dy -D_g^k \frac{\partial}{\partial z} \phi_g^k(x,y,z) \Big|_{z=\pm \Delta z^k/2} \quad (7)$$

THE TRANSVERSE INTEGRATION PROCEDURE IN HEXAGONAL GEOMETRY

The equations for the face-averaged partial currents required for the evaluation of the leakages in Eq. (2) are derived via an extension to hexagonal geometry of the transverse integration procedure⁵ widely used in the development of Cartesian-geometry nodal schemes. In Cartesian geometry this technique involves spatially integrating the n-dimensional diffusion equation over the n-1 directions transverse to each coordinate direction. The resulting set of n coupled ordinary differential equations are approximated using techniques appropriate for the numerical solution of the one-dimensional diffusion equation. Additional approximations to the transverse-leakage terms which couple the one-dimensional equations are also required.

Direct application of the analogous transverse integration procedure in three-dimensional hexagonal geometry yields four second-order ordinary differential equations in the x-, u-, v-, and z-directions. However, a more straightforward procedure is to derive the P-1 forms of these equations using simple neutron balance arguments. For example, the one-dimensional equation in the x-direction is obtained by first introducing the partially-integrated quantities

$$\phi_{gx}^k(x) \equiv \int_{-\Delta z^k/2}^{\Delta z^k/2} dz \int_{-y_s(x)}^{y_s(x)} dy \phi_g^k(x,y,z), \quad (8)$$

$$J_{gx}^k(x) \equiv \int_{-\Delta z^k/2}^{\Delta z^k/2} dz \int_{-y_s(x)}^{y_s(x)} dy -D_g^k \frac{\partial}{\partial x} \phi_g^k(x, y, z), \quad (9)$$

and then performing a neutron balance on the two-dimensional slice (perpendicular to the x-direction) defined by

$$\delta V^k: (x, y, z) \quad x \in [x, x + dx], \quad y \in [-y_s(x), +y_s(x)], \quad z \in [-\Delta z^k/2, +\Delta z^k/2].$$

The result is

$$\frac{d}{dx} J_{gx}^k(x) + \Sigma_g^{r,k} \phi_{gx}^k(x) = Q_{gx}^k(x) - \frac{2}{\sqrt{3}} [J_{gxy}^k(x, y_s(x)) - J_{gxy}^k(x, -y_s(x))] - \int_{-y_s(x)}^{y_s(x)} dy L_{gz}^k(x, y). \quad (10)$$

The terms $J_{gx}^k(x, \pm y_s(x))$ are z-integrated, surface-normal components of the net currents across the u- and v-directed surfaces:

$$J_{gxy}^k(x, \pm y_s(x)) \equiv \int_{-\Delta z^k/2}^{\Delta z^k/2} dz -D_g^k \hat{n}_{\pm} \cdot \nabla \phi_g^k(x, y, z) \Big|_{y=\pm y_s(x)}, \quad (11)$$

where

$$\hat{n}_{+} \equiv \begin{cases} \hat{n}_{v+} & -h/2 < x < 0 \\ \hat{n}_{u+} & 0 < x < h/2 \end{cases}, \quad \hat{n}_{-} \equiv \begin{cases} \hat{n}_{u-} & -h/2 < x < 0 \\ \hat{n}_{v-} & 0 < x < h/2 \end{cases},$$

and, for example, \hat{n}_{v+} denotes the unit vector normal to the surface in the positive v-direction shown in Figure 1. The final term in Eq. (10) involves the z-direction leakage

$$L_{gz}^k(x,y) \equiv \int_{-\Delta z^k/2}^{\Delta z^k/2} dz -D_g^k \frac{\partial^2}{\partial z^2} \phi_g^k(x,y,z). \quad (12)$$

Integration of Eq. (10) over $x \in [-h/2, +h/2]$ yields the nodal balance equation, as it should.

Since Eq. (10) is in P-1 form, we require an additional equation (analogous to Fick's Law) relating the partially-integrated flux and net current. This relationship is derived by differentiating Eq. (8) and rearranging:

$$J_{gx}^k(x) \equiv -D_g^k \frac{d}{dx} \phi_{gx}^k(x) + D_g^k y_s'(x) [\phi_{gxy}^k(x, y_s(x)) + \phi_{gxy}^k(x, -y_s(x))], \quad (13)$$

where

$$\phi_{gxy}^k(x,y) \equiv \int_{-\Delta z^k/2}^{\Delta z^k/2} dz \phi_g^k(x,y,z), \quad (14)$$

$$y_s'(x) = -\frac{1}{\sqrt{3}} \operatorname{sgn}(x). \quad (15)$$

The u- and v-direction counterparts to Eqs. (10) and (13) are derived in an analogous manner.

The one-dimensional equation in the z-direction can be derived either by integrating the three-dimensional diffusion equation over the x- and y-directions, or by performing a neutron balance over a two-dimensional slice perpendicular to the z-direction. The result is

$$\frac{d}{dz} J_{gz}^k(z) + \Sigma_g^{r,k} \phi_{gz}^k(z) = Q_{gz}^k(z) - L_{gxy}^k(z), \quad (16)$$

where

$$\phi_{gz}^k(z) \equiv \int_{-h/2}^{h/2} dx \int_{-y_s(x)}^{y_s(x)} dy \phi_g^k(x,y,z), \quad (17)$$

$$J_{gz}^k(z) = -D_g^k \frac{d}{dz} \phi_{gz}^k(z), \quad (18)$$

$$L_{gxy}^k(z) \equiv \int_{-h/2}^{h/2} dx \int_{-y_s(x)}^{y_s(x)} dy -D_g^k \left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right] \phi_g^k(x, y, z). \quad (19)$$

The total hex-plane leakage is

$$\begin{aligned} \bar{L}_{gxy}^k &\equiv \frac{3h}{2} \frac{1}{v^k} \int_{-\Delta z^k/2}^{\Delta z^k/2} dz L_{gxy}^k(z) \\ &\equiv \bar{L}_{gx}^k + \bar{L}_{gu}^k + \bar{L}_{gv}^k. \end{aligned} \quad (20)$$

As before, integration of Eq. (16) over $z \in [-\Delta z^k/2, +\Delta z^k/2]$ yields the nodal balance equation.

It is clear that the partially-integrated net currents introduced in Eqs. (9) and (18) must be continuous over the respective one-dimensional intervals. Therefore, with reference to Eqs. (13) and (15), it is also clear that the partially-integrated fluxes in the three hex-plane directions will exhibit first-derivative discontinuities of the form

$$\lim_{\epsilon \rightarrow 0} [-D_g^k \frac{d}{dx} \phi_{gx}^k(x)]_{x=-\epsilon}^{x=\epsilon} = \frac{2D_g^k}{\sqrt{3}} [\phi_{gxy}^k(x, y_s(x)) + \phi_{gxy}^k(x, -y_s(x))]_{x=0}. \quad (21)$$

This behavior, which does not appear in Cartesian geometry, must be represented by any polynomial used to approximate $\phi_{gx}^k(x)$.

APPROXIMATION OF THE ONE-DIMENSIONAL HEX-PLANE EQUATIONS

The partially-integrated fluxes in the three hex-plane directions are approximated by

$$\phi_{gx}^k(x) \equiv 2y_s(x) [\bar{\phi}_g^k + \sum_{n=1}^4 a_{gxn}^k f_n(x)], \quad (22)$$

where

$$a_{gx1}^k \equiv \bar{\phi}_{gx}^k(+h/2) - \bar{\phi}_{gx}^k(-h/2) \quad (23)$$

$$a_{gx2}^k \equiv \bar{\phi}_{gx}^k(+h/2) + \bar{\phi}_{gx}^k(-h/2) - 2\bar{\phi}_g^k \quad (24)$$

$$f_1(x) \equiv \frac{x}{h} \equiv \xi \quad (25a)$$

$$f_2(x) \equiv \frac{36}{13} \xi^2 - \frac{5}{26} \quad (25b)$$

$$f_3(x) \equiv \frac{10}{13} \xi^2 - \frac{1}{2} |\xi| + \frac{3}{52} \quad (25c)$$

$$f_4(x) \equiv \xi (|\xi| - \frac{1}{2}). \quad (25d)$$

Here, $\bar{\phi}_{gx}^k(\pm h/2)$ denotes the two face-averaged fluxes in the x -direction, and the basis functions satisfy

$$\int_{-h/2}^{h/2} dx \, 2y_s(x) f_n(x) \equiv 0, \quad n=1, \dots, 4; \quad (26a)$$

$$f_n(\pm h/2) \equiv 0, \quad n=3, 4. \quad (26b)$$

Note that $f_3(x)$ has a first-derivative discontinuity at $x=0$.

The expansion coefficient a_{gx3}^k is calculated in the following manner. Requiring that Eq. (22) satisfy Eq. (21) yields

$$a_{gx3}^k \equiv E_{gx}^k(0), \quad (27)$$

where

$$E_{gx}^k(x) \equiv \phi_{gxy}^k(x, y_s(x)) + \phi_{gxy}^k(x, -y_s(x)) - 2 \left[\frac{1}{2y_s(x)} \phi_{gx}^k(x) \right]. \quad (28)$$

Expanding $\phi_{gxy}^k(x, y)$ in a Taylor series about $y=0$ yields

$$E_{gx}^k(x) = - \frac{1}{6D_g^k} [2y_s(x)]^2 \dot{x}_{gy}^k(x) + O(h^4), \quad (29)$$

where

$$\dot{x}_{gy}^k(x) \equiv \int_{-\Delta z^k/2}^{\Delta z^k/2} dz \frac{1}{2y_s(x)} \int_{-y_s(x)}^{y_s(x)} dy -D_g^k \frac{\partial^2}{\partial y^2} \phi_g^k(x, y, z). \quad (30)$$

The y-direction leakage $\dot{x}_{gy}^k(x)$ is approximated by its respective averages over the half-intervals $-h/2 < x < 0$ and $0 < x < h/2$. These average values are calculated in terms of average leakages in the u- and v-directions by requiring that the x-dependent net currents defined in Eq. (11) satisfy the constraints

$$\frac{2}{h} \int_{-h/2}^0 dx [J_{gxy}^k(x, y_s(x)) - J_{gxy}^k(x, -y_s(x))] \equiv \bar{J}_{gv}^k(+h/2) - \bar{J}_{gu}^k(-h/2) \quad (31a)$$

$$\frac{2}{h} \int_0^{h/2} dx [J_{gxy}^k(x, y_s(x)) - J_{gxy}^k(x, -y_s(x))] \equiv \bar{J}_{gu}^k(+h/2) - \bar{J}_{gv}^k(-h/2). \quad (31b)$$

This calculation⁹ leads to an expression for a_{gx3}^k which is used to eliminate the expansion coefficient from the final equations.

The expansion coefficient a_{gx4}^k is calculated by applying a weighted residual procedure to Eq. (10) with weight function $w_x(x) \equiv \text{sgn}(x)$. This procedure, when applied in the x-, u-, and v-directions, is equivalent to preserving a neutron balance over each pair of half-nodes in the three directions. The coefficient a_{gx4}^k is eliminated from the final equations in favor of the x-direction flux moment

$$\phi_{gx1}^k \equiv \frac{1}{v^k} \int_{-\Delta z^k/2}^{\Delta z^k/2} dz \int_{-h/2}^{h/2} dx w_x(x) \int_{-y_g(x)}^{y_g(x)} dy \phi_g^k(x, y, z). \quad (32)$$

APPROXIMATION OF THE ONE-DIMENSIONAL AXIAL EQUATION

The partially-integrated flux [Eq. (17)] in the axial direction is approximated by a cubic polynomial equivalent to that used to approximate the one-dimensional fluxes in the Cartesian-geometry nodal expansion method.¹⁰ The cubic coefficient is computed using a weighted residual approximation to Eq. (16) with weight function $w_z(z) \equiv z/\Delta z^k$. As in the hex-plane approximation, this coefficient is eliminated in favor of the spatial moment

$$\phi_{gz1}^k \equiv \frac{1}{v^k} \int_{-\Delta z^k/2}^{\Delta z^k/2} dz w_z(z) \int_{-h/2}^{h/2} dx \int_{-y_g(x)}^{y_g(x)} dy \phi_g^k(x, y, z). \quad (33)$$

THE RESPONSE MATRIX EQUATION

Using the polynomial approximations to the partially-integrated fluxes in the hex-plane and axial directions, equations for the face-averaged outgoing partial currents on the eight surfaces of the hexagonal-z node can be derived. Combining results in the four directions yields the inhomogeneous response matrix equation for the k-th node and g-th energy group:

$$\underline{J}_g^{\text{out},k} = [P_g^k] \{ \underline{Q}_g^k - \underline{L}_g^k \} + [R_g^k] \underline{J}_g^{\text{in},k}. \quad (34)$$

The vectors $\underline{J}_g^{\text{out},k}$ and $\underline{J}_g^{\text{in},k}$ contain, respectively, the eight outgoing and eight incoming face-averaged partial currents for the node. The source-moment vector is calculated using

$$\underline{Q}_g^k = \frac{1}{\lambda} \chi_g \sum_{g'=1}^G v \Sigma_{g'}^{f,k} \phi_{g'}^k + \sum_{g' \neq g} \Sigma_{gg'}^{s,k} \phi_{g'}^k, \quad (35)$$

where

$$\phi_g^k = \text{col} [\bar{\phi}_g^k, \phi_{gx1}^k, \phi_{gul}^k, \phi_{gvl}^k, \phi_{gz1}^k]. \quad (36)$$

The leakage-moment vector is

$$\underline{L}_g^k = \text{col} [0, \frac{1}{\Delta z^k} L_{gzx1}^k, \frac{1}{\Delta z^k} L_{gzul}^k, \frac{1}{\Delta z^k} L_{gzvl}^k, \frac{2}{3h} L_{gxyz1}^k], \quad (37)$$

where L_{gzx1}^k and L_{gxyz1}^k are spatial moments [analogous to Eqs. (32) and (33)] of the leakages defined in Eqs. (12) and (19), respectively. The local source ($[P_g^k]$) and response ($[R_g^k]$) matrices involve a combined total of 13 unique entries for each node and each group. However, since these entries depend only upon the material properties and axial mesh spacing for the k-th node, they are pre-computed and stored only for unique nodes characterized by material composition assignment and axial mesh spacing.

The transverse leakage moments [Eq. (37)] are computed using the following simple approximations to Eqs. (12) and (19):

$$L_{gz}^k(x,y) \approx \bar{L}_{gz}^k, \quad (38)$$

$$L_{gxy}^k(z) \approx \rho_{gxy}^k(z), \quad (39)$$

where $\rho_{gxy}^k(z)$ is a quadratic polynomial¹⁰ involving the total hex-plane leakages [Eq. (20)] in the k-th node and its two immediate neighbors in the axial direction. Use of Eq. (38) yields

$$L_{gzx1}^k \approx L_{gzul}^k \approx L_{gzvl}^k \approx 0, \quad (40)$$

while use of Eq. (39) permits evaluation of L_{gxyz1}^k in terms of the available partial currents in the k-th node and its immediate axial neighbors.

NUMERICAL SOLUTION OF THE NODAL EQUATIONS

The response matrix and flux-moment equations are solved using a conventional fission source iteration accelerated by coarse-mesh rebalance¹¹ and asymptotic source extrapolation.¹² The rebalance is performed on a mesh such that each ring of hexagons forms a hex-plane rebalance zone. The response matrix equations are solved at each outer iteration using two axial sweeps (for each energy group) of the mesh planes in a standard checkerboard ordering. The hex-plane partial

currents for each plane are computed using a "four-color checkerboard" sweep in which all outgoing hex-plane partial currents from nodes not sharing a common surface are solved simultaneously at each of four passes through the nodes on the plane. Two such sweeps are typically performed on each plane encountered during the axial sweeps. The outgoing z-directed partial currents are then computed using a single sequential sweep of the nodes on the plane. Once all partial currents for a single group have been computed in this manner, the spatial flux moments are updated using the nodal balance equation and the moments equations generated via the weighted residual approximations.

NUMERICAL RESULTS

Numerical results at the beginning of cycle 1 (BOC1) for a 4-group version of the three-dimensional Large Core Code Evaluation Working Group (LCCEWG) benchmark problem¹³ are summarized in Table 1. This problem is a model of a 1000 MWe heterogeneous-core design with 17 rings of hexagons and a lattice pitch of 16.33 cm. Shown in Table 1 are results obtained using the nodal scheme, which has been implemented as an option⁹ in the fast-reactor diffusion-theory code DIF3D (Ref. 1), as well as results calculated using the highly-optimized mesh-centered finite difference option with 6 and 24 triangular mesh cells per hexagonal assembly. The 14-plane mesh structure uses an axial mesh spacing of 15.24 cm in the driver fuel, and is the coarsest mesh permitted by the axial zone boundaries used to define the burnup regions. Extrapolated results assuming an infinite number of axial planes have been included in order to allow isolation of the errors due to the respective axial approximations. Using these extrapolated results, it can be seen that the errors in eigenvalue due to the axial approximation are greater in the 56-plane finite difference calculations than in the 14-plane nodal calculation. Comparison of the axially-converged (∞ -plane) calculations shows that the nodal option produces somewhat larger (but very acceptable) errors in the driver fuel, but yields significantly smaller errors in eigenvalue and in the internal and radial blankets than the DIF3D(6A) calculation. Although the overall accuracy of the 14-plane nodal calculation is superior to that of the 56-plane DIF3D(6A) calculation, the nodal calculation required a factor of 9 less computing time with a reduction in dollar cost by a factor of nearly 12. The reduction in job cost reflects the reduced core storage requirements and I/O activity for the nodal option in addition to the smaller CPU time.

Depletion calculations¹³ using the DIF3D nodal option have shown that the improved accuracy in the computed eigenvalues and internal blanket fluxes leads in turn to significantly improved predictions of the reactivity swing due to burnup. REBUS-3 (Ref. 3) burnup calculations¹⁴ using DIF3D nodal and finite-difference neutronics solutions are summarized in Table 2. The excellent agreement between the burnup swings computed using the DIF3D(NODAL) and DIF3D(24A) options confirms the improved accuracy of the nodal method relative to the conventional 6 triangles-per-hexagon finite difference scheme.

CONCLUSIONS

The results presented in the previous section (plus additional results given in Refs. 9 and 13) have shown the accuracy of the nodal scheme to be superior to that of the standard 6 triangles-per-hexagon finite difference method. The higher-order axial approximation in the nodal scheme permits the use of an axial mesh which is at least 4 times coarser than that used in a typical finite difference calculation. Particular improvement is seen in the average fluxes in the internal blanket regions and in the computed values for k -effective, thus leading to more accurate predictions of internal blanket burnups, breeding ratios, and burnup reactivity swings. This enhanced accuracy is obtained with a potential order-of-magnitude reduction in the computational cost of a three-dimensional calculation. The accuracy and computational efficiency of the nodal scheme will make possible the development of an efficient three-dimensional hexagonal-geometry kinetics capability for the analysis of LMFBR transients.

REFERENCES

- 1 D. R. Ferguson and K. L. Derstine, "Optimized Iteration Strategies and Data Management Considerations for Fast Reactor Finite Difference Diffusion Theory Codes," Nucl. Sci. Engr., 64, 593 (1977).
- 2 C. H. Adams, "SYN3D - A Single-Channel, Spatial Flux Synthesis Code for Diffusion Theory Calculations," ANL-76-21, Argonne National Laboratory, 1976.
- 3 B. J. Toppel, "The Fuel Cycle Analysis Capability, REBUS-3", Argonne National Laboratory, in preparation.
- 4 A. F. Henry, "Refinements in Accuracy of Coarse-Mesh Finite-Difference Solution of the Group Diffusion Equations," in Numerical Reactor Calculations, p. 447, International Atomic Energy Agency, Vienna (1972).
- 5 See for example: J. Dorning, "Modern Coarse-Mesh Methods - A Development of the 70's," Proceedings of the Topical Meeting on Computational Methods in Nuclear Engineering, Williamsburg, VA, Vol. 1, p. 3-2, American Nuclear Society, April, 1979.
- 6 T. Duracz, "A Nodal Method in Hexagonal Geometry," Proceedings of the International Topical Meeting on Advances in Mathematical Method for the Solution of Nuclear Engineering Problems, Munich, Vol. 1, p. 423, American Nuclear Society/European Nuclear Society, April, 1981.
- 7 J. J. Arkuszewski, and M. Makai, "Analytical Coarse Mesh Approximations for Solving Diffusion Equations in Hexagonal and Square Geometries," Proceedings of the International Topical Meeting on Advances in Mathematical Methods for the Solution of Nuclear Engineering Problems, Munich, Vol. 2, p. 89, American Nuclear Society/European Nuclear Society, April 1981.

- 8 R. D. Lawrence, "A Nodal Interface Current Method for Multigroup Diffusion Calculations in Hexagonal Geometry," Trans. Am. Nucl. Soc., 39, 461 (1981).
- 9 R. D. Lawrence, "The DIF3D Nodal Neutronics Option for Two- and Three-Dimensional Diffusion Theory Calculations in Hexagonal Geometry," Argonne National Laboratory, in preparation.
- 10 H. Finnemann, F. Bennewitz, and M. R. Wagner, "Interface Current Techniques for Multidimensional Reactor Calculations," Atomkernenergie, 30, 123 (1977).
- 11 R. Froehlich, "A Theoretical Foundation for Coarse-Mesh Variational Techniques," GA-7870, Gulf General Atomic, 1968.
- 12 M. R. Wagner, "GAUGE - A Two-Dimensional Few Group Neutron Diffusion-Depletion Program for A Uniform Triangular Mesh," GA-8307, Gulf General Atomic, 1968.
- 13 B. J. Toppel, C. H. Adams, R. D. Lawrence, H. Henryson II, and K. L. Derstine, "Validation of Alternative Methods and Data for a Benchmark Fast Reactor Depletion Calculation," Proceedings of the Topical Meeting on Advances in Reactor Physics and Core Thermal Hydraulics, Kiamesha Lake, NY, NUREG/CP-0034, Vol. 1, p. 177, U.S. Nuclear Regulatory Commission, Washington DC, August, 1982.
- 14 B. J. Toppel, Private Communication, 1982.

Table 1. Summary of BOC1 Results for the Three-Dimensional LCCEWG Problem^a

Method	No. of Axial Planes	k-eff	ϵ_k (%)	ϵ_{DF} (%)	ϵ_{IB} (%)	ϵ_{RB} (%)	ϵ_{AB} (%)	CPU Time ^c (min)	Cost (\$)
DIF3D(NODAL)	14	0.9985	0.15	1.4	3.1	0.8	2.3	1.1	7.28
DIF3D(NODAL)	28	0.9983	0.13	1.6	3.2	0.7	1.6	2.5	18.29
DIF3D(NODAL)	∞	0.9982	0.12	1.6	3.2	0.7	1.5	---	---
DIF3D(6 Δ)	28	1.0033	0.63	0.8	4.2	3.4	5.3	5.3	43.14
DIF3D(6 Δ)	56	1.0021	0.51	0.7	4.4	3.1	2.1	10.2	85.27
DIF3D(6 Δ)	∞	1.0017	0.47	0.7	4.4	3.0	1.0	---	---
DIF3D(24 Δ)	28	0.9998	0.28	0.5	1.1	1.3	4.9	30.5	336.72
DIF3D(24 Δ)	56	0.9986	0.16	0.2	1.1	0.8	1.3	59.0	674.00
DIF3D(24 Δ)	∞	0.9981	0.11	0.1	1.1	0.6	0.1	---	---
Reference ^b	∞	0.9970	---	---	---	---	---	---	---

^a ϵ_k \equiv error in k-effective

ϵ_{DF} \equiv average error in region-averaged power density over driver fuel regions.

ϵ_{IB} \equiv average error in region-averaged power density over internal blanket regions.

ϵ_{RB} \equiv average error in region-averaged power density over radial blanket regions.

ϵ_{AB} \equiv average error in region-averaged power density over axial blanket regions.

^b Reference solution obtained by h^2 extrapolation of DIF3D(6 Δ) - 28 plane and DIF3D(24 Δ) - 56 plane calculations.

^c IBM 3033 Computer using sixth-core planar symmetry.

Table 2. Computed Burnup Swings for the Three-Dimensional LCCEWG Benchmark Problem^a

Method	No. of Axial Planes	Burnup Swing (Δk)	Neutronics CPU Time ^b (min)
DIF3D(NODAL)	17	-0.00426	2.6
DIF3D(6 Δ)	42	-0.00489	14.0
DIF3D(24 Δ)	42	-0.00420	81.1

^aThe burnup swings are for the first half of a 388.5 day cycle.

^bIBM 3033.

Figure 1. Nodal Coordinate System

