High-Order Finite Difference Nodal Method for Neutron Diffusion Equation

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A nodal method has been developed which accurately and rapidly solves the three-dimensional neutron diffusion equation in both Cartesian and hexagonal geometries.

To reduce the number of unknowns in comparison with the interface current method in favor of short computation time and a small computer memory requirement, this method employs the finite difference method (FDM) as its global neutron balance solution method. In the global neutron balance solution, the coupling coefficients are modified in such a way as to conserve the nodal interface neutron currents which are obtained by a local neutron balance solution method fit to each geometry.

To validate the method developed here, it has been applied to neutron diffusion calculations for reactor cores, typical of Cartesian and hexagonal geometries, with different core sizes, assembly pitches, core configurations, control rod patterns, etc. For a large FBR (hexagonal geometry), for example, errors in power distribution and control rod worth by the method are less than 1/2 and 1/10, respectively, compared to an ordinary FBR core design method, while the computation time is 1/8 that of the latter method.

KEYWORDS: neutron diffusion equation, finite difference method, nodal method, accuracy, Cartesian geometry, hexagonal geometry, computation time, computer memory, power distribution, control rod worths, FBR type reactors, PWR type reactors

I. INTRODUCTION

Reliable design of nuclear reactors requires accurate prediction of the three-dimensional power and exposure distributions within the reactor core. This often requires a three-dimensional neutron diffusion calculation using an enormous number of spatial meshes. Such a calculation naturally requires a long computation time and a large computer memory even for static problems, making its application to kinetics analysis impractical. For this reason, from early days many nodal methods have been developed for efficient neutron diffusion calculations(1). A homogenization method for taking account of spatial heterogeneity by using discontinuity factors(2)(3), which make it possible to reproduce heterogeneous transport calculation results with good accuracy within the bounds of homogeneous diffusion theory, has particularly enhanced the recent development of nodal methods.

The nodal methods have a common characteristic which is that the three-dimensional neutron flux distribution is iteratively calculated by solving in turns two kinds of neutron balance, local and global. In the local neutron balance solution, neutron flux distribution in each node (or coarse spatial mesh) is determined by using information from the global neutron balance solution, i.e., node average neutron fluxes and/or interface neutron currents. The local neutron balance solution results are fed back to the global neutron balance solution for better accuracy. Thus, a high accuracy can be attained with a small number of nodes without drastically increasing computation time. Computation times required by recent methods in Cartesian geometry are reported to be less than 1/100 those of fine-mesh finite difference methods (FDMs) with the same
accuracy\(^{(1)}\).

The nodal methods, depending on how the global neutron balance is solved, can be classified into two types, the interface current method (ICM) type and the finite difference method (FDM) type. Most nodal methods these days are of the former type, in which the global neutron balance is solved by the ICM. The ICM treats as unknowns partial neutron currents across node interfaces as well as node average neutron fluxes. It requires several times larger computer memory compared to the FDM which treats only node average neutron fluxes\(^{(4)}\). This disadvantage of the ICM type is never a minor problem in analyzing some types of nuclear reactors such as fast breeder reactors, which require multigroup theory and in turn need large computer memory. In addition, most nodal methods of the ICM type\(^{(5)}\)\(^{(6)}\) yield less satisfying accuracy in hexagonal geometry than in Cartesian geometry because of poor approximations regarding the transverse leakage distribution in the former geometry.

The FDM type\(^{(7)}\)\(^{(11)}\) treats as unknowns only node average neutron fluxes in the global neutron balance solution. Therefore, it is thought to be more advantageous than the ICM type from the viewpoint of attaining a high accuracy with limited computer memory and computation time. In addition to this, conventional FDM resources and numerical techniques are available for this type, requiring less code development cost. The methods described in Refs.\(^{(7)}\)\(^{(11)}\), however, have lower accuracy than the ICM-type methods due to rough approximations used in the local neutron balance solution.

The purpose of this paper is to propose a new FDM-type nodal method which requires less computer memory than the ICM-type methods and provides satisfying accuracy in both Cartesian and hexagonal geometries within a short computation time.

II. OUTLINE OF FDM-TYPE NODAL METHOD

In the method proposed here, the global neutron balance is solved by the FDM, in which the coupling coefficients are modified in such a way as to conserve neutron current obtained by local neutron balance solution. In the local neutron balance solution, the neutron current across each node interface is calculated by a method fit to each geometry. Described below are the outlines of the global and local neutron balance solutions, the latter of which is explained for Cartesian and hexagonal geometries in different sections.

One-group theory is employed for simplicity; its extension to multigroup theory is straightforward. For the same reason, an equal mesh division is assumed in each coordinate direction; its extension to general cases is also straightforward.

1. Global Neutron Balance Solution

In the global neutron balance solution, the initial guess values of node average neutron fluxes are calculated by an ordinary (first-order) FDM. These guess values are then used to get neutron current across each node interface with more rigorous models in the local neutron balance solution, details of which are described in the following sections. The recalculated neutron current is fed back to the global neutron balance solution to recalculate the node average neutron fluxes.

To do this within the bounds of the FDM, the coupling coefficients (coefficients of node average neutron fluxes appearing in the neutron current term) are modified after each local neutron balance solution. That is, in the global neutron balance solution, a finite difference type balance equation is solved using a slightly modified expression for neutron current.

\[
\sum_{j} S_{ij} J_{ij} + \left( \Sigma_{a_{ij}} - \frac{\nu \Sigma_{f_{ij}}}{k_{eq}} \right) \phi_i V_i = 0 \quad (1)
\]

\[
J_{ij} = \frac{1}{h} \left( \frac{2D_i D_j}{D_i + D_j} + \delta D_{ij} \right) \phi_i \]

\[
- \left( \frac{2D_i D_j}{D_i + D_j} - \delta D_{ij} \right) \phi_j \quad (2)
\]

Here \( h \) is the mesh spacing between nodes \( i \) and \( j \); \( D_i, \Sigma_{a_{ij}} \) and \( \nu \Sigma_{f_{ij}} \) the macroscopic group constants in node \( i \); \( V_i \) the node volume; \( S_{ij} \) the interface area between nodes \( i \) and \( j \);
\( \bar{\phi}_i \) and \( J_{ij} \) the node average neutron flux in node \( i \) and neutron current between nodes \( i \) and \( j \), respectively; \( k_{\text{eff}} \) the effective multiplication factor.

The quantity \( \delta D_{ij} \) in Eq. (2) is modified after each local neutron balance solution so that the equation using the existing node average neutron fluxes \( \bar{\phi}_i \) and \( \bar{\phi}_j \) reproduces the neutron current which is obtained in the local neutron balance solution.

As shown above, the main characteristic of the proposed method is that high-order spatial effects are treated by a nonlinear FDM. For this reason, the method is hereafter referred to as a high-order finite difference nodal method (HFM); the same classification was employed by Lawrence in his review paper(1).

2. Local Neutron Balance Solution in Cartesian Geometry

The local neutron balance equations of the HFM in Cartesian geometry, like those of many other nodal methods, can be derived from the equivalent one-dimensional diffusion equation which is obtained by transverse integrating the three-dimensional neutron diffusion equation. The equivalent one-dimensional diffusion equation along the \( x \)-direction, for instance, can be written in the following form:

\[
D_i \frac{d^2 \Psi_i}{d x^2} - \sum_{a} \Psi_i + \frac{\nu}{k_{\text{eff}}} \Psi_i + L_i(x) = 0.
\]  
\[
(3)
\]

Here \( \Psi_i(x) \) and \( L_i(x) \) are the quantities defined by

\[
\Psi_i(x) = \int_{-h_y/2}^{h_y/2} \int_{-h_z/2}^{h_z/2} d y \, d z \, \phi(x, y, z),
\]
\[
L_i(x) = \int_{-h_y/2}^{h_y/2} \int_{-h_z/2}^{h_z/2} d y \, d z \left( \frac{\partial \phi}{\partial z} \bigg|_{x=x_i, z=z_{i-1/2}} - \frac{\partial \phi}{\partial z} \bigg|_{x=x_i, z=-z_{i+1/2}} \right).
\]
\[
(4)
\]

The origin of the spatial coordinates \( x, y \) and \( z \) is taken to be at the center of the node interface as shown in Fig. 1: \( \phi(x, y, z) \) is the neutron flux; \( h_y \) and \( h_z \) are the node lengths in the \( y \)- and \( z \)-directions, respectively. The external source term \( L_i(x) \) corresponds to transverse neutron leakage across the node interfaces, which is approximated by fitting to a second-order polynomial the average transverse leakages of three consecutive nodes.

![Neutron flux distribution over two adjacent nodes in Cartesian geometry](Fig. 1)

Here, by employing an analytical technique(13), the general solution to Eq. (3) is expressed by

\[
\Psi_i(x) = C_{i,1} \sin \beta_i x + C_{i,2} \cos \beta_i x + S_i(x),
\]
\[
(5)
\]

where \( S_i(x) \) is the special solution term resulting from the external neutron source term \( L_i(x) \); \( C_{i,1} \) and \( C_{i,2} \) the unknown constants to be so determined that \( \Psi_i(x) \) should have a physical meaning; \( \beta_i \) the square root of material buckling.

In the local neutron balance solution, Eq. (3) is solved over two adjacent nodes \( i \) and \( j \) (i.e., region \([-h_x, h_x]\) in Fig. 1). This means that four algebraic equations per energy group are necessary to determine all the unknown constants appearing in the two nodes, i.e., \( C_{i,1}, C_{i,2}, C_{j,1} \) and \( C_{j,2} \).

These four equations can be derived from the following requirements.

1. Neutron flux must be continuous at the node interface.
\[
\Psi_i(0) = \Psi_j(0)
\]
\[
(7)
\]

2. Neutron current must also be continuous at the node interface.
Average neutron fluxes in the adjacent nodes \( i \) and \( j \) must be equal to the neutron flux values \( \bar{\phi}_i \) and \( \bar{\phi}_j \); respectively, given beforehand by the global neutron balance solution based on the FDM.

Thus, the coefficients \( C_{i1} \) and \( C_{i2} \) can be determined by solving the simultaneous algebraic equations derived from Eqs. (7)-(10), which coefficients determine neutron flux distribution \( \Psi_i(x) \). In consequence, neutron current across the node interface can be calculated by

\[
 J_{ij} = -D_i \frac{d\Psi_i}{dx} \bigg|_{x=0} \quad \text{ (11)}
\]

This neutron current is fed back to the global neutron balance solution, i.e. its value is used in Eq. (2) to calculate \( \delta D_{ij} \).

The neutron currents in the \( y \)- and \( z \)-directions are obtained in the same manner as that in the \( x \)-direction.

No mention has been made for simplicity about the use of discontinuity factors for taking account of heterogeneity. It can be easily treated by only multiplying the neutron fluxes by the discontinuity factors in Eq. (7).

### 3. Local Neutron Balance Solution in Hexagonal Geometry

The transverse integration method as described in the last section yields satisfying results in Cartesian geometry. However, it is not as successful in hexagonal geometry as in Cartesian geometry. This is because the equivalent one-dimensional diffusion equation is difficult to solve accurately in hexagonal geometry, and also because transverse leakage cannot be well approximated by a polynomial fit.

In a complicated geometry like hexagonal nodes, division of each node into many triangular regions, as in finite element methods, often leads to a much simpler treatment than analytical and/or polynomial methods; information regarding the transverse neutron leakage distribution is not necessarily required. For this reason, a fine-mesh FDM has been employed to derive the local neutron balance equations for hexagonal geometry. Explained below is the derivation of the radial balance equations.

In solving a local neutron balance, each node is first subdivided into six triangular meshes as shown in Fig. 2.

![Fig. 2 Mesh division of hexagonal nodes](image-url)

Then, the finite difference type neutron balance equations are derived for the two triangular meshes bordering the node interface.

\[
 \frac{3D_i}{\sqrt{3}} (\phi_i^* - \phi_{i2}^*) - \frac{3D_i}{\sqrt{3}} (\phi_i^* - \phi_{i6}^*) = \frac{h}{\sqrt{3}} J_{ij} \quad \text{(12a)}
\]

\[
 \frac{\nu \Sigma f_{ij}}{k_{eff}} - \frac{\nu \Sigma a_{ij} - D_i \beta_{ij}}{k_{eff}} \phi_{i2}^* \frac{h^2}{4 \sqrt{3}} = 0 \quad \text{(12b)}
\]

\[
 J_{ij} = \frac{6D_i D_j}{h(D_i + D_j)} (\gamma_{ij} \phi_{i2}^* - \gamma_{ij} \phi_{j2}^*) \quad \text{(13)}
\]

Here \( \phi_{ik}^* \) is the average neutron flux in the \( k \)-th triangular mesh in node \( i \); \( h \) the assembly pitch and \( \beta_{ij} \) the axial neutron buckling calculated from the axial neutron flux distribution in the case of three-dimensional problems. The factor \( \gamma_{ij} \) is designed to correct for spatial mesh effects resulting from the
use of triangular meshes. Its principle is explained later.

Simultaneous equations (12) and (13) involve too many unknowns to solve. Therefore, an assumption is made that the mesh average neutron fluxes $\tilde{\phi}_{ik}$ change linearly in each node. Then, $\tilde{\phi}_{i2}$ and $\tilde{\phi}_{i6}$ satisfy the following relation:

$$\frac{\tilde{\phi}_{i2} + \tilde{\phi}_{i6}}{2} = \frac{\tilde{\phi}_{i} + \tilde{\phi}_{i1}}{2}, \quad (14)$$

where $\tilde{\phi}_{i}$ is the average neutron flux in node $i$;

$$\tilde{\phi}_{i} = \frac{1}{6} \sum_{k=1}^{6} \phi_{ik}. \quad (15)$$

Substitution of Eqs. (13) and (14) into Eq. (12) leads to

$$-\frac{3D_{1}}{h}(\tilde{\phi}_{i2} - \tilde{\phi}_{i}) - \frac{6D_{1}D_{j}}{h(D_{1} + D_{j})}(\gamma_{r}, \tilde{\phi}_{i1}^{*} - \gamma_{j}, \tilde{\phi}_{j1}^{*})$$

$$+ \left( \nu \sum_{j} \frac{1}{k_{\text{eff}}} - \Sigma_{ai} - D_{i} \beta_{ai} \right) \tilde{\phi}_{i1}^{*} \frac{h}{4} = 0, \quad (16a)$$

$$-\frac{3D_{2}}{h}(\tilde{\phi}_{i6} - \tilde{\phi}_{j}) - \frac{6D_{1}D_{j}}{h(D_{1} + D_{j})}(\gamma_{r}, \tilde{\phi}_{j1}^{*} - \gamma_{r}, \tilde{\phi}_{i1}^{*})$$

$$+ \left( \nu \sum_{j} \frac{1}{k_{\text{eff}}} - \Sigma_{aj} - D_{j} \beta_{aj} \right) \tilde{\phi}_{j1}^{*} \frac{h}{4} = 0. \quad (16b)$$

Neutron balance equation (16) takes into account transverse neutron leakage within the bounds of the FDM using six triangular meshes per hexagonal node. Node average neutron fluxes $\tilde{\phi}_{i}$ and $\tilde{\phi}_{j}$ are given by the global neutron balance solution. Therefore, simultaneous equations (16) can be solved in terms of $\tilde{\phi}_{i1}$ and $\tilde{\phi}_{j1}$ to get neutron current $J_{ij}$, which is fed back to the global neutron balance solution (i.e., it is used in Eq. (2) to calculate $\delta D_{i}$) in the same manner as in Cartesian geometry.

In describing the neutron current between adjacent nodes in Eq. (13), $\tilde{\phi}_{i1}$ is multiplied by a correction factor $\gamma_{ir}$ to get an accurate neutron flux gradient at the node interface. As shown in Fig. 3, this factor is defined as the ratio of the imaginary neutron flux at the triangular mesh center obtained by extrapolation from the neutron flux and its gradient at the node interface to the mesh average value. Concretely, it is given by

$$\gamma_{ir} = \frac{\Phi_{i}(y) \left( \frac{h}{2} - \frac{h}{6} \frac{d \Phi_{i}}{dx} \right)_{x = h/6}}{\int_{x = h/6}^{x = h/3} \frac{h}{x} \Phi_{i}(x) \, dx},$$

where $\Phi_{i}(x)$ is neutron flux distribution within the triangular mesh and $x$ the distance from the node center in the direction of adjacent node $j$. The neutron flux $\Phi_{i}(x)$ can be assumed to be a cosine or hyperbolic cosine function, for instance, using material buckling $\beta_{i}^{*}$. The expression for $\beta_{i}^{*}$ in multigroup theory is shown in Refs. (9) and (11). This value is also recalculated.

The axial neutron balance equations are the same as those derived by Komano, et al., except that neutron fluxes are multiplied by correction factors similar to $\gamma_{ir}$ and transverse (i.e., radial) neutron leakage is considered.

No mention has been made for simplicity about the use of discontinuity factors. It can be easily incorporated in the same manner as described in Ref. (13).

III. NUMERICAL TEST CALCULATIONS

1. Test Calculations in Cartesian Geometry

To evaluate the applicability of the HFM
to Cartesian geometry, it has been applied to the two-dimensional benchmark PWR core\(^{18}\) as shown in Fig. 4. For comparison the two-group diffusion calculation was performed also by the FDM with fine mesh divisions. Figure 5 shows a comparison of the results. The reference values are the same as those used in Ref. (12). The listed data from the HFM with one node per assembly are quite satisfactory, i.e., its power distribution agrees within 1% with the reference. This accuracy is almost equivalent to that of the FDM with 20×20 meshes per assembly; the FDM with 10×10 meshes per assembly yields an error of as much as 3%. These results show that the FDM requires over 100 times more computation time and computer memory than the HFM with the same accuracy, because the HFM requires only three times as much computation time as the coarse-mesh FDM with one node per assembly.

The accuracy of the HFM naturally increases with the number of nodes used for each assembly. Though not listed here, it was confirmed that the power distribution by the HFM with 2×2 nodes per assembly deviated by only 0.3% from the reference.

The HFM has also been applied to other types of reactor cores such as those of BWRs and ATR-type HWRs (pressure-tube-type heavy water reactors) with different assembly pitches (15-24 cm), CR patterns (CR-in and CR-out) and burnup states (beginning of cycle and end of cycle; flat exposure distribution was assumed in each node). In all these cases, radial power distribution by the HFM yielded calculational results as satisfactory as those of the recent nodal methods employing the ICM.

2. Test Calculations in Hexagonal Geometry

To validate the HFM in hexagonal geometry, it has been applied to three-dimensional six-group neutron diffusion calculations for the 1,000-MWe homogeneous fast breeder reactor (FBR) core as shown in Fig. 6. This was chosen because of its large fuel assembly pitch (16.4 cm), which makes it difficult to obtain a high accuracy by the diffusion calculation using hexagonal nodes. In performing the calculation, axial mesh spacings were chosen such that they were about the same

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**Fig. 4** Configuration of benchmark PWR core

**Fig. 5** Comparison of percent errors in benchmark PWR power distribution
as the radial mesh spacing. For comparison, three-dimensional power distribution has been calculated also by a fine-mesh calculation (FMC: FDM using 24 meshes per assembly) and by a triangular mesh calculation (TMC: FDM using 6 meshes per assembly). The latter is often performed for FBR core design calculation. The number of axial meshes used in the TMC and FMC were double and quadruple, respectively, that of the HMF. These calculations were performed with the CITATION program (14).

Using the FMC as a reference, differences in assembly powers in the driver core region between the HFM and TMC are shown in Fig. 7. In the core with all control rods (CRs) withdrawn, both methods provide sufficient accuracy; the difference is less than 0.5%. In the case of 13 CRs (central and all the outermost CRs) being fully inserted, on the other hand, there is an appreciable difference between the two methods; power distribution by the HFM deviates by less than 2%, while that by the TMC is greater than 4%. This constitutes an overall decrease in error of less than half when comparing the HFM with the TMC.

Differences in effective multiplication factor $k_{\text{eff}}$ and CR worth are also reduced to less than half and 1/10 those of the TMC, respectively, as shown in Table 1.

Table 1 Comparison of $k_{\text{eff}}$ and CR worth in 1,000-MWe FBR core

<table>
<thead>
<tr>
<th>Method</th>
<th>$k_{\text{eff}}$</th>
<th>CR-out</th>
<th>CR-in</th>
<th>$% \Delta k/k_{\text{eff}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>FMC</td>
<td>1.03244</td>
<td>0.97060</td>
<td>6.17</td>
<td>(13 CRs)</td>
</tr>
<tr>
<td>TMC</td>
<td>1.03399(0.155)</td>
<td>0.97547(0.487)</td>
<td>5.8(−5.8)</td>
<td></td>
</tr>
<tr>
<td>HFM</td>
<td>1.03312(0.068)</td>
<td>0.97123(0.063)</td>
<td>6.17(0.0)</td>
<td></td>
</tr>
</tbody>
</table>

† Percent differences from FMC

Besides the above example, the HFM has also been applied to FBR cores with different assembly pitches (11–18 cm), CR patterns, core sizes (600–1,300 MWe) core configurations (homogeneous and heterogeneous cores), etc.
In all these cases much the same results as above have been obtained.

Computation time of the HFM is only 1/8 that required by the TMC.

IV. CONCLUSION

A nodal method for the solution of the three-dimensional neutron diffusion equation in Cartesian and hexagonal geometries has been developed and numerically tested. The new, high-order finite difference nodal method (HFM) employs as its global neutron balance solution method the finite difference method (FDM) to reduce the number of unknowns to less than that of the interface current method in favor of short computation time and a small computer memory requirement. To retain a high accuracy, the coupling coefficients are modified such that neutron currents obtained by the local neutron balance solution can be conserved. In the local neutron balance solution, the neutron currents are calculated by a method fit to each geometry.

The neutron diffusion calculation results for a variety of FBR, PWR, BWR and HWR cores have shown that the HFM is efficient in both Cartesian and hexagonal geometries. It particularly yields satisfactory results for large FBR cores; errors of power distribution and control rod worth by the HFM are less than half and less than 1/10, respectively, compared to an ordinary FBR core design method, i.e., the FDM with six triangular meshes per assembly. The computation time of the HFM is about 1/8 that of the latter method.

The small computer memory requirement of the HFM makes it possible to perform large-scale, three-dimensional diffusion calculations for a greater variety of purposes than ever, such as space kinetics and on-line core performance calculations. Since it is based on the FDM, the HFM has another practical merit, i.e., conventional FDM resources and numerical techniques can be utilized, reducing cost, time and manpower for code development.

REFERENCES