M&C 2001 Salt Lake City, Utah, USA, September 2001.

Nonlinear Unified Nodal Method Formulation for Analytic Function Expansion Nodal Method Solution to Two-Group Diffusion Equation in Rectangular Geometry

Hyun Chul Lee and Chang Hyo Kim
Nuclear Engineering Department, Seoul National University
San 56-1 Shillim-dong, Kwanak-gu, Seoul, 151-742, Korea
lhc@sniper9.snu.ac.kr kchyo@snu.ac.kr

Keywords: Nonlinear unified nodal method, Analytic function expansion nodal method, One-node nonlinear nodal iteration scheme, Two-node nonlinear nodal iteration scheme

ABSTRACT

Nonlinear unified nodal method (UNM) formulation for the analytic function expansion nodal (AFEN) method solutions to the two-group (2-G) diffusion equation in rectangular geometry is presented. A one-node nonlinear UNM scheme is newly proposed. Its computational effectiveness is compared with those of a two-parameter, two-node nonlinear UNM and conventional UNM which does not utilize nonlinear kernels in terms of nodal solutions to IAEA and OECD L336 neutronics benchmark problems. It is shown that the nonlinear UNM formulation can speed up the iterative solution process of the original AFEN method and that the one-node nonlinear UNM scheme is far more efficient than the two-node nonlinear UNM scheme and the original AFEN formulation, judging from the computational time of each method. The advantages of the UNM formulation for the AFEN method solution over the original AFEN method are then discussed.

1. INTRODUCTION

The unified nodal method (UNM) was originally introduced to show (Lee,2001) that the analytic nodal method (ANM) solution to two-group (2-G) diffusion equation in rectangular geometry can be formulated in exactly the same way as the nodal expansion method (NEM) by representing the analytic solution of transverse integrated 2-G diffusion equations by an expansion of basis functions similar to those of the NEM (Finnemann,1977) and thereby to demonstrate that the two most popular transverse integrated nodal methods (TINM), NEM (Finnemann,1977) and ANM (Smith,1979), can be integrated into a single unified formulation. Recently, we demonstrated that the analytic function expansion nodal (AFEN) method (Noh,1994) can also be integrated into the UNM by using the principle of the UNM formulation (Lee,2000)(Lee,2000). The purpose of this paper is to present the nonlinear UNM formulation of the AFEN option and examine its computational effectiveness in terms of numerical solutions to the IAEA (Argonne Code Center, 1977) and OECD-L336 MOX (Lefebvre,1977) core neutronics

benchmark problems. We show that the non-linear nodal schemes (Smith,1983) (Turinsky,1994) (Joo,1998) designed for speedy nodal method calculations are also applicable to the UNM calculation of the AFEN option. In particular, we present a one-node nonlinear scheme as an alternative to the popular two-node scheme and show that the one-node scheme is more effective than the two-node scheme for speedy UNM calculations through numerical tests.

2. UNM FORMULATION OF AFEN METHOD

The UNM formulation for the AFEN calculations are presented in some detail in reference (Lee,2000). At the risk of repeating it, however, we summarize here some of major steps in the UNM formulation of the AFEN option. Then we present the nonlinear iterative schemes available for enhancement of the computational efficiency.

The AFEN method is based on the following intranodal flux distribution:

$$\begin{aligned}\xi_p(x,y) \cong\ & A_{p0} + A_{p1}\sinh\kappa_p x + A_{p2}\cosh\kappa_p x + A_{p3}\sinh\kappa_p y + A_{p4}\cosh\kappa_p y \\ & + B_{p1}\sinh\frac{\kappa_p}{\sqrt{2}}x\sinh\frac{\kappa_p}{\sqrt{2}}y + B_{p2}\sinh\frac{\kappa_p}{\sqrt{2}}x\cosh\frac{\kappa_p}{\sqrt{2}}y \\ & + B_{p3}\cosh\frac{\kappa_p}{\sqrt{2}}x\sinh\frac{\kappa_p}{\sqrt{2}}y + B_{p4}\cosh\frac{\kappa_p}{\sqrt{2}}x\cosh\frac{\kappa_p}{\sqrt{2}}y\end{aligned} \quad , \qquad (1)$$

which is an approximate solution to the decoupled reactor eigenvalue equations of the 2-G diffusion equation,

$$\nabla^2\boldsymbol{\xi}_p(x,y) - \lambda_p\boldsymbol{\xi}_p(x,y) = 0\,;\ p = 1,2\,. \qquad (2)$$

The 2-G flux vector, $\boldsymbol{\phi}$ =column vector ($\phi_1(x,y)$, $\phi_2(x,y)$), is related to $\boldsymbol{\xi}$ =column vector ($\xi_1(x,y)$, $\xi_2(x,y)$) by $\boldsymbol{\phi} = \mathbf{R}\boldsymbol{\xi}$ in which $\mathbf{R}$ is the similarity transformation matrix. The nine coefficients are determined by nine nodal unknowns per node per neutron group: node average flux, four nodal surface fluxes and four corner point fluxes of the given rectangular node. The use of the nodal balance relation, current continuity conditions along four nodal interfaces, and four corner point balance (CPB) relations leads to the nodal coupling relations among nodal unknowns (Noh,1994). This way of deriving nodal coupling relations are quite different from that of TINM. The coupling relations of AFEN method resemble none of TINM. In reference (Lee,2000) however, we showed that, aside from the relations for four corner point fluxes, which are not nodal unknowns of TINM, the remaining coupling equations can be put in exactly same form as NEM in our UNM formulation.

To show this, let us perform the transverse integration of Eq. (2) to obtain;

$$\frac{d^2}{du^2}\xi_{pu}(u) - \lambda_p\xi_{pu}(u) = \hat{L}_{pu}(u)\,. \qquad (3)$$

The $\xi_{pu}(u) = \frac{1}{a_u}\int_{-a_u/2}^{+a_u/2}\xi_p(u,v)dv$ and $\hat{L}_{pu}(u) = -\frac{1}{a_u}\int_{-a_u/2}^{+a_u/2}\frac{\partial^2}{\partial v^2}\xi_p(u,v)dv$ are the transverse integrated 1-D flux and the transverse leakage, respectively. Because of Eq. (1) for the intranodal flux $\xi_p(x,y)$, $\hat{L}_{pu}(u)$ can be expressed by

$$\hat{L}_{pu}(u) = \sum_{i=0}^{2}\hat{L}_{ipu}g_{ipu}(u), \tag{4}$$

where $g_{0pu}(u) = 1$, $g_{1pu}(u) = a_1\sinh\left(\kappa_p u/\sqrt{2}\right)$, and $g_{2pu}(u) = a_2\cosh\left(\kappa_p u/\sqrt{2}\right) + b_2$ and a_1, a_2, b_2 are determined so that $g_{1pu}(\pm a_u/2) = \pm 1$, $g_{2pu}(\pm a_u/2) = +1$, and $\int_{-a_u/2}^{+a_u/2}g_{ipu}(u)du = 0$ $(i = 1,2)$. $\hat{L}_{ipu}$ $(i = 0,1,2)$ are given by corner point ($\xi_p^i; i = 1,2,3,4$), surface average (ξ_{pus}; $u = x, y$, $s = r, l$), and node average value ($\bar{\xi}$) of $\xi_p(x,y)$. For example, $\hat{L}_{2pu}$ is given by

$$\hat{L}_{2pu} = \frac{\rho_{p2}}{8(1-\rho_{p2})}\left(\xi_p^{(1)} + \xi_p^{(2)} + \xi_p^{(3)} + \xi_p^{(4)} + 4\bar{\xi} - 2\xi_{pxr} - 2\xi_{pxl} - 2\xi_{pyr} - 2\xi_{pyl}\right);$$

$$\rho_{p2} = \frac{2\sqrt{2}}{\kappa_p a_u}\tanh\frac{\kappa_p a_u}{2\sqrt{2}}, \ (p = 1,2) \tag{5}$$

Instead of using $\xi_{pu}(u)$ from direct integration of $\xi(u,v)$ over v, the UNM formulation uses the analytic solution of Eq. (3) which can be obtained by assuming the following expansion,

$$\xi_{pu}(u) = \sum_{i=0}^{4}\hat{C}_{ipu}f_{ipu}(u/a_u), \tag{6}$$

where the basis functions $f_{ipu}(\tau)$ are given in reference (Lee,2000) and are chosen so that they have the same properties as the polynomial basis functions, $h_i(\tau)$, of the NEM. The $\hat{C}_{ipu}$ of $\xi_{pu}(u)$ are determined by nodal balance condition, $\bar{\xi}_p = 1/a_u\int_{-a_u/2}^{+a_u/2}\xi_{pu}(u)du$, two conditions at two nodal surfaces, $\xi_{pu}(\pm a_u/2)$, and two weighted residual method (WRM) equations:

$$\int_{-a_u/2}^{+a_u/2}f_{ipu}(u/a_u)\left[\text{Eq. (3) with } \xi_{pu}(u) \text{ in Eq. (6)}\right]du, \quad i = 1,2. \tag{7}$$

Reference (Lee,2001) describes the algebraic details on how to determine the $\hat{C}_{ipu}$, the two-group flux vector from $\boldsymbol{\phi} = \mathbf{R}\boldsymbol{\xi}$, and the nodal coupling relations between node

average fluxes, and partial currents. Following the procedure of reference (Lee,2001), one can find the following nodal coupling relations:

$$\bar{\boldsymbol{\phi}} = (\mathbf{A} + 12\mathbf{Q}_0)^{-1}\mathbf{S}\,, \tag{8.a}$$

$$\mathbf{j}_{ur}^{+} = \mathbf{Q}_{0u}\left(6\bar{\boldsymbol{\phi}} - \mathbf{C}_{4u}\right) - \mathbf{Q}_{1u}\mathbf{C}_{3u} - \mathbf{Q}_{2u}\mathbf{j}_{ul}^{+} + \mathbf{Q}_{3u}\mathbf{j}_{ur}^{-}\,, \tag{8.b}$$

$$\mathbf{j}_{ul}^{-} = \mathbf{Q}_{0u}(6\bar{\boldsymbol{\phi}} + \mathbf{C}_{4u}) + \mathbf{Q}_{1u}\mathbf{C}_{3u} - \mathbf{Q}_{2u}\mathbf{j}_{ur}^{-} + \mathbf{Q}_{3u}\mathbf{j}_{ul}^{+}\,, \tag{8.c}$$

where

$$\mathbf{S} = \sum_{u=x,y,z} \frac{2\mathbf{Q}_{0u}\mathbf{C}_{4u} + \left(\mathbf{I} + \mathbf{Q}_{2u} - \mathbf{Q}_{3u}\right)\left(\mathbf{j}_{ur}^{-} + \mathbf{j}_{ul}^{+}\right)}{a_u}, \tag{9}$$

$$\mathbf{C}_{3u} = \mathbf{R}\hat{\mathbf{C}}_{3u} = \mathbf{M}_{3u}^{-1}(\mathbf{M}_{1u}\mathbf{C}_{1u} + \mathbf{L}_{1u})\,, \tag{10.a}$$

$$\mathbf{C}_{4u} = \mathbf{R}\hat{\mathbf{C}}_{4u} = \mathbf{M}_{4u}^{-1}(\mathbf{M}_{2u}\mathbf{C}_{2u} + \mathbf{L}_{2u})\,, \tag{10.b}$$

$$\mathbf{M}_{1u} = \mathbf{R}\hat{\mathbf{A}}\hat{\mathbf{H}}_{3u}\mathbf{R}^{-1}, \quad \mathbf{M}_{3u} = \mathbf{D}\mathbf{R}\hat{\mathbf{G}}_{3u}\hat{\mathbf{H}}_{3u}\mathbf{R}^{-1},$$

$$\mathbf{M}_{2u} = \mathbf{R}\hat{\mathbf{A}}\hat{\mathbf{H}}_{4u}\mathbf{R}^{-1}, \quad \mathbf{M}_{4u} = \mathbf{D}\mathbf{R}\hat{\mathbf{G}}_{4u}\hat{\mathbf{H}}_{4u}\mathbf{R}^{-1},$$

$$\mathbf{L}_{iu} = \mathbf{D}\mathbf{R}\hat{\mathbf{L}}_{iu} \quad (i = 1,2)$$

The equations (8) correspond to nodal balance relations, and relations between incoming and outgoing partial currents. They constitute the basic nodal coupling relations in the UNM formulations. Depending on NEM, ANM or AFEN option, the diagonal matrices $\hat{\mathbf{G}}_{iu}$ and $\hat{\mathbf{H}}_{iu}\,(i = 3,4)$ and vector $\mathbf{L}_{iu}\,(i = 1,2)$ are differently defined. In the AFEN option, $\mathbf{L}_{2u}$, for example, is given by nine nodal unknown fluxes of the given node;

$$\mathbf{L}_{2u} = \mathbf{P}_v\left[\boldsymbol{\phi}^{(1)} + \boldsymbol{\phi}^{(2)} + \boldsymbol{\phi}^{(3)} + \boldsymbol{\phi}^{(4)} + 4\bar{\boldsymbol{\phi}} - 2\left(\boldsymbol{\phi}_{ur} + \boldsymbol{\phi}_{ul} + \boldsymbol{\phi}_{vr} + \boldsymbol{\phi}_{vl}\right)\right]\left(u = x, y; v = y, x\right) \tag{11}$$

Because the coefficients $\mathbf{L}_{iu}\,(i = 1,2)$ are given by corner point fluxes, extra relations are needed for corner point fluxes. One can use the five point relations derived from the corner point leakage balance (CPB) condition (Noh,1994);

$$\mathbf{T}_i^C\boldsymbol{\phi}_{ij} + \mathbf{T}_{ij}^L\boldsymbol{\phi}_{ij} + \mathbf{T}_{ij}^R\boldsymbol{\phi}_{ij} + \mathbf{T}_{ij}^B\boldsymbol{\phi}_{ij} + \mathbf{T}_{ij}^T\boldsymbol{\phi}_{ij} = \mathbf{q}_{ij}\,. \tag{12}$$

Equation (13) is the extra relation in the AFEN option of the UNM formulation.

Equation (8) in combination with Eqs. (10), and (12) constitute a set of the basic nodal coupling relations in the UNM formulation. Except for Eq. (12), they are practically the same as those in the NEM formulation. In order to solve these relations, therefore, one can use the same iterative procedure introduced in reference (Finnemann,1977) for NEM. Alternatively, one can utilize nonlinear coarse mesh finite difference (CMFD) schemes that will be described next.

3. NONLINEAR UNM SOLUTION SCHEMES

The nonlinear nodal schemes that have been used for speedy nodal solution are also applicable to the AFEN option of UNM formulation with a slight modification. The nonlinear UNM scheme here consists of representing both the net current, J_{gu}^{m}, and the surface average flux, ϕ_{gu}^{m}, on the interface *m* of the two adjacent nodes by node average fluxes of the left and the right nodes as follows:

$$J_{gu}^{m} = -\frac{2\beta_{gu}^{r}\beta_{gu}^{l}}{\beta_{gu}^{r}+\beta_{gu}^{l}}\left(\bar{\phi}_{gu}^{r}-\bar{\phi}_{gu}^{l}\right)-D_{g}^{N}\left(\bar{\phi}_{gu}^{r}+\bar{\phi}_{gu}^{l}\right), \tag{13a}$$

$$\phi_{gu}^{m} = \frac{\beta_{gu}^{r}\bar{\phi}_{gu}^{r}+\beta_{gu}^{l}\bar{\phi}_{gu}^{l}}{\beta_{gu}^{r}+\beta_{gu}^{l}}-\Gamma_{g}^{N}\left(\bar{\phi}_{gu}^{r}+\bar{\phi}_{gu}^{l}\right), \tag{13b}$$

where $\beta_{gu}^{s} = D_{g}^{s}/a_{u}^{s}\left(s=l,r\right)$. The first terms of Eq. (13) correspond to the finite difference approximations to J_{gu}^{m} and ϕ_{gu}^{m}, respectively. The second terms are designed for correction of the finite difference approximation. D_{g}^{N} and Γ_{g}^{N} are corrective coupling coefficients for J_{gu}^{m} and ϕ_{gu}^{m}, respectively, which are to be iteratively updated as the nonlinear scheme dictates. In case of the TINM, only Eq. (13a) is used (Joo,1998) for transforming the nodal balance equation into the mesh centered coarse-mesh finite difference (CMFD) equation for the unknown node average fluxes. In case of the AFEN option, however, ϕ_{gu}^{m} need also be updated by Eq.(13b) because ϕ_{gu}^{m} is contained in the source term of the CPB equations and in the vectors, $\mathbf{L}_{iu}\left(i=1,2\right)$, of the WRM equations for $\mathbf{C}_{iu}\left(i=3,4\right)$. There can be a variation of nonlinear UNM schemes, depending on how to determine J_{gu}^{m} and ϕ_{gu}^{m}. Here we introduce two nonlinear schemes; one-node and two-node nonlinear schemes.

3.1 One-Node Nonlinear Nodal Iteration Scheme

The one-node CMFD scheme was first introduced by Shin et al. (1999) in conjunction with transforming fine-mesh finite difference equations into the CMFD equations. The main idea of the one-node scheme here comes from this. Unlike the two-node scheme that will be described in the following section, one-node scheme does not introduce any new equations. Instead, it makes the most of the nodal coupling relations,

Eqs. (8b) and (8c) , in determining the updated J_{gu}^{m} and ϕ_{gu}^{m} as noted in the following algorithm.

1. Set $D_g^N = \Gamma_g^N = 0$
2. Use Eq. (13a) to form a mesh centered CMFD equation, and solve the CMFD equation for new node average fluxes of all the computational nodes.
3. Obtain new J_{gu}^{m} and ϕ_{gu}^{m} for all the nodes using Eq. (13) with new node average fluxes and then use them to determine partial currents by

$$j_{gu}^{m\pm} = \frac{1}{4}\phi_{gu}^{m} \pm \frac{1}{2}J_{gu}^{m}$$

4. Solve the CPB equations to update the corner point fluxes and thus update $\mathbf{L}_{iu}$ and $\mathbf{C}_{iu}$ in turn.
5. Update the node average fluxes using Eq. (8a) and the outgoing partial currents using the nodal coupling equations (8b) and (8c). In this step all the computational nodes are swept through one by one.
6. Repeat step 5 two to three times to further update $\bar{\phi}_g$ and $j_{gu}^{m\pm}$ based on Eqs. (8a), (8b), and (8c)
7. Determine the new J_{gu}^{m} and ϕ_{gu}^{m} by

$$J_{gu}^{m} = j_{gu}^{m+} - j_{gu}^{m-}, \quad \phi_{gu}^{m} = 2\left(j_{gu}^{m+} + j_{gu}^{m-}\right)$$

8. Update D_g^N and Γ_g^N and go to step 2.

The one node algorithm described above is fit for the AFEN option of the UNM calculations. Needless to mention, however, it is also applicable to the TINM option with minor modifications.

3.2 Two-node Nonlinear Nodal Iteration Scheme

Two-node nonlinear scheme has been applied to the TINM (Turinsky,1994) (Joo,1998) and the original AFEN (Moon,1999). In order to determine J_{gu}^{m} and ϕ_{gu}^{m} and thus update parameters D_g^N and Γ_g^N, it utilizes the solution to the two-node 1-D, 2-G diffusion equations defined by

$$\frac{d^2}{du^2}\boldsymbol{\xi}_{\mathrm{u}}^{\mathrm{s}}(u) = \hat{\mathbf{A}}^{s}\boldsymbol{\xi}_{\mathrm{u}}^{\mathrm{s}}(u) + \hat{\mathbf{L}}_{u}^{s}(u) \quad (s = l, r), \tag{14a}$$

or $$\frac{d^2}{du^2}\xi_{pu}^{s}(u) = \lambda_p^s \xi_{pu}^{s}(u) + \hat{L}_{pu}^{s}(u) \quad (p = 1,2). \tag{14b}$$

The parameters superscripted with $s(=l,r)$ denote those corresponding to the left node $(s=l)$ and the right node $(s=r)$, respectively. For the solution to Eq. (14), the 1-D fluxes are represented by an expansion like Eq.(6) for each node,

$$\xi_{pu}^{s}(u)=\sum_{i=0}^{4}\hat{C}_{ipu}^{s}f_{ipu}^{s}\left(u/a_{u}^{s}\right)\ (p=1,2;s=l,r)\,. \tag{15}$$

The above expansion contains five unknown coefficients for each region, $\hat{C}_{iu}^{s}\left(i=0,1,\cdots,4;s=l,r\right)$. Defining $\mathbf{C}_{iu}^{s}\equiv\mathbf{R}^{s}\hat{\mathbf{C}}_{iu}^{s}\ \ (i=0,1,2,3,4)$ and noting $\mathbf{C}_{0u}^{s}=\overline{\boldsymbol{\phi}}_{u}^{s}$, one can determine $\mathbf{C}_{iu}^{s}\ (i=1,2,3,4)$ by using the nodal balance equation for each node, flux and current continuity conditions at the interface of the two-nodes, and two WRM equations each node shown below :

(i) nodal balance equation

$$\int_{-a_u/2}^{+a_u/2}\left[\text{Eq.(14b) with }\xi_{pu}^{s}(u)\text{ replaced by Eq. (15)}\right]du\ \ (s=l,r) \tag{16}$$

$$\text{or}\ \ 12\mathbf{B}_{u}^{s}\mathbf{C}_{2u}^{s}+2\mathbf{B}_{u}^{s}\mathbf{C}_{4u}^{s}=a_{u}^{s}\left(\mathbf{A}^{s}\mathbf{C}_{0u}^{s}+\mathbf{L}_{0u}^{s}\right)\quad (s=l,r), \tag{17}$$

(ii) flux continuity equation

$$\mathbf{C}_{1u}^{l}+\mathbf{C}_{1u}^{r}=\left(\mathbf{C}_{0u}^{r}+\mathbf{C}_{2u}^{r}\right)-\left(\mathbf{C}_{0u}^{l}+\mathbf{C}_{2u}^{l}\right), \tag{18}$$

(iii) current continuity equation

$$\mathbf{B}_{u}^{l}\left(2\mathbf{C}_{1u}^{l}+\mathbf{C}_{3u}^{l}\right)-\mathbf{B}_{u}^{r}\left(2\mathbf{C}_{1u}^{r}+\mathbf{C}_{3u}^{r}\right)=-\mathbf{B}_{u}^{l}\left(6\mathbf{C}_{2u}^{l}+\mathbf{C}_{4u}^{l}\right)-\mathbf{B}_{u}^{r}\left(6\mathbf{C}_{2u}^{r}+\mathbf{C}_{4u}^{r}\right), \tag{19}$$

(iv) the first moment WRM equation

$$-\mathbf{M}_{1u}^{s}\mathbf{C}_{1u}^{s}+\mathbf{M}_{3u}^{s}\mathbf{C}_{3u}^{s}=\mathbf{L}_{1u}^{s}\quad (s=l,r), \tag{20}$$

(v) the second moment WRM equation

$$-\mathbf{M}_{2u}^{s}\mathbf{C}_{2u}^{s}+\mathbf{M}_{4u}^{s}\mathbf{C}_{4u}^{s}=\mathbf{L}_{2u}^{s}\quad (s=l,r), \tag{21}$$

where $\mathbf{L}_{0u}^{s}=\left(\mathbf{J}_{vr}^{s}-\mathbf{J}_{vl}^{s}\right)/a_{u}$ and $\mathbf{B}_{u}^{s}=\mathbf{D}^{s}/a_{u}$

Equations (17) to (21) form a closed set of equations for determining eight unknown vectors, $\mathbf{C}_{iu}^{s}\ (i=1,2,3,4)$. One can determine $\mathbf{C}_{2u}^{s}$ and $\mathbf{C}_{4u}^{s}(s=l,r)$ from solving Eqs. (17) and (21). Equation (20) relates $\mathbf{C}_{3u}^{s}$ to $\mathbf{C}_{1u}^{s}$. The substitution of this result into Eq. (19) leads to equation containing the two unknown coefficients $\mathbf{C}_{1u}^{s}(s=l,r)$, which can be readily solved for $\mathbf{C}_{1u}^{s}$ by combining with Eq.(18). Once they are determined, it is

a straightforward matter to determine J_{gu}^{m} and ϕ_{gu}^{m} from $\mathbf{C}_{iu}^{s}$ $(i=1,2,3,4)$ and update D_g^N and Γ_g^N from Eqs. (13a) and (13b) in turn. Nonlinear iteration schemes described above require solving the CMFD equations with node average fluxes as unknowns. For accelerated iterative solution of the CMFD equations, the bi-conjugate gradient stabilized (BICGSTAB) algorithm (Saad,1996) and the Wielandt method (Fladmark,1972) are employed.

In the UNM calculation of the AFEN option, one need to determine $\mathbf{L}_{iu}$ $(i=1,2)$ using the corner point fluxes from the solution of the CPB equation (12). For numerical enumeration, however, one must take precaution against the direct use of Eq. (11). Equation (11) is poorly conditioned because subtraction of large flux values is involved in determining the transverse leakage expansion coefficients that are smaller in numerical value by an order than fluxes. Therefore, use of $\mathbf{L}_{iu}$ (i=0,1,2) determined directly from substituting large but inaccurate flux values from intermediate iteration stages into Eq. (11) may lead to erroneous results or fail to produce the converged solution. As will be discussed later, we face non-convergence difficulty in 3-D applications and fine-mesh UNM calculations of the AFEN option. This appears a drawback of the UNM formulation for the AFEN method. But the non-convergence difficulty can be easily avoided by enumerating $\mathbf{L}_{iu}$ using an under-relaxation scheme as follows;

$$\mathbf{L}_{iu}^{new} = \mathbf{L}_{iu}^{old} + \omega \left(\mathbf{L}_{iu} - \mathbf{L}_{iu}^{old} \right) \quad (i=0,1,2) \tag{22}$$

where $\mathbf{L}_{iu}^{new}$ and $\mathbf{L}_{iu}^{old}$ are transverse leakage coefficients of the current and the previous steps, respectively. $\mathbf{L}_{iu}$ is the transverse leakage coefficients determined directly from Eq.(12) using flux values of the current step. ω (< 1) is the relaxation parameter.

4. NUMERICAL RESULTS AND DISCUSSIONS

Aside from the CPB equation (12), the nodal coupling equations (8a), (8b) and (8c) of our UNM formulation are equivalent to those of the original AFEN formulation presented by Noh et al.(1994), even though they look very different from Noh's AFEN counterpart. Accordingly, our UNM and Noh's AFEN formulations must produce the identical solution to the 2-G neutronics problems. Figure 1 compares the UNM and the original AFEN computations for the effective multiplication factor (k_{eff}) and the normalized fuel assembly (FA) power densities of the IAEA 2-D neutronics benchmark problem. The UNM and the AFEN computations here are obtained with the zero incoming boundary condition that is originally imposed for the IAEA 2-D problem. For the comparison of two computations, two different flux convergence criteria, 10^{-5} and 10^{-7}, are applied. It is shown that, with the flux convergence criterion of 10^{-5}, the UNM and AFEN calculations have the discrepancies in FA power densities in the fourth significant digit but that, with the convergence criterion of 10^{-7}, the FA power densities of two calculations agree with each other to the fourth significant digit. As for k_{eff}, two calculations predict the same values regardless of the two different convergence criteria.

These results manifest the fact that our UNM and the original AFEN method are indeed identical, even though the two formulations have little or no resemblance in the nodal coupling equations, except for the CPB equations.

(a) Flux Convergence Criteria = 10^{-5}

0.7456	1.3097	1.4537	1.2107	0.6100	0.9351	0.9343	0.7549
0.7445	1.3049	1.4486	1.2067	0.6097	0.9334	0.9338	0.7547
0.7443	1.3047	1.4484	1.2066	0.6098	0.9337	0.9342	0.7550
	1.4351	1.4351	1.3149	1.0697	1.0361	0.9504	0.7358
	1.4320	1.4320	1.3129	1.0669	1.0356	0.9511	0.7358
	1.4319	1.4319	1.3130	1.0671	1.0360	0.9515	0.7362
		1.4694	1.3451	1.1792	1.0705	0.9752	0.6921
		1.4684	1.3441	1.1767	1.0713	0.9749	0.6952
		1.4685	1.3443	1.1770	1.0717	0.9754	0.6955
			1.1929	0.9670	0.9064	0.8461	
			1.1918	0.9653	0.9078	0.8512	
			1.1922	0.9656	0.9082	0.8516	
				0.4706	0.6856	0.5972	
				0.4713	0.6847	0.6023	
				0.4715	0.6851	0.6026	
					0.5849		
					0.5903		
					0.5906		

k-eff	
1.02959	Reference
1.02961	AFEN
1.02961	UAFEN

(b) Flux Convergence Criteria = 10^{-7}

0.7456	1.3097	1.4537	1.2107	0.6100	0.9351	0.9343	0.7549
0.7445	1.3050	1.4487	1.2068	0.6098	0.9336	0.9340	0.7548
0.7445	1.3050	1.4487	1.2068	0.6098	0.9336	0.9340	0.7548
	1.4351	1.4799	1.3149	1.0697	1.0361	0.9504	0.7358
	1.4322	1.4780	1.3132	1.0671	1.0359	0.9513	0.7361
	1.4322	1.4780	1.3132	1.0671	1.0359	0.9513	0.7361
		1.4694	1.3451	1.1792	1.0705	0.9752	0.6921
		1.4687	1.3444	1.1770	1.0716	0.9752	0.6954
		1.4687	1.3444	1.1770	1.0716	0.9752	0.6954
			1.1929	0.9670	0.9064	0.8461	
			1.1922	0.9656	0.9081	0.8515	
			1.1922	0.9656	0.9081	0.8515	
				0.4706	0.6856	0.5972	
				0.4715	0.6850	0.6025	
				0.4715	0.6850	0.6025	
					0.5849		
					0.5906		
					0.5906		

k-eff	
1.02959	Reference
1.02961	AFEN
1.02961	UAFEN

Figure 1 Comparison of the UNM and the original AFEN method calculation for IAEA-2D neutronics benchmark problem

The UNM formulation provides a good opportunity to compare the computational effectiveness of various nodal options on an equal footing because one solves practically the same set of nodal coupling relations in the UNM formulation for solutions to the 2-G neutronics problems in rectangular geometry. Tables 1-3 compare the prediction accuracy of five different nodal computational options of our UNM formulation in terms of 1 node-per-assembly (N/A) calculations for k_{eff} normalized FA power density, and thermal and fast fluxes in 2-D and 3-D IAEA PWR and OECD-L336 C3 and C5 MOX cores. NEM/QPA and ANM/QPA are the NEM and ANM solutions with quadratic polynomial transverse leakage approximation(QPA), respectively. ANM/ATL is the ANM solution with analytic transverse leakage determined by Eq. (4), of which the expansion

coefficients are determined in the same way as QPA(Lee,2000). There are two AFEN solutions: AFEN/MSS and AFEN/CPB. In the AFEN/MSS the corner point fluxes are determined by the method of successive smoothing (MSS) (Fischer,1981), while in the AFEN/CPB they are determined by the CPB equation (12). As observed in previous studies, the numerical results in these tables show that the AFEN is the most accurate. Two AFEN options show similar prediction accuracy in FA power density and node average fluxes. AFEN/CPB appears to predict k_{eff} slightly more accurately than AFEN/MSS. The NEM is the least accurate. The ANM/QPA is more accurate than the NEM but is less accurate than the ANM/ATL. The accuracy of the ANM/ATL is slightly lower than, but compares very well with, that of the AFEN method.

Table 1. Comparison of UNM solutions to IAEA 2-D benchmark problems

UNM Options	Δk_{eff} pcm	FA power density error, %		Node average fast flux error, %		Node average thermal flux error, %	
		$\varepsilon_{\max}^{a)}$	$\varepsilon_{rms}^{b)}$	$\varepsilon_{\max}^{a)}$	$\varepsilon_{rms}^{b)}$	$\varepsilon_{\max}^{a)}$	$\varepsilon_{rms}^{b)}$
NEM/QPA	-5.9	1.45	0.73	1.60	0.70	1.45	0.72
ANM/QPA	+5.1	1.57	0.58	0.66	0.32	1.55	0.57
ANM/ATL	+2.6	0.90	0.33	0.35	0.17	0.90	0.32
AFEN/MSS	-8.3	0.69	0.27	0.59	0.30	0.67	0.26
AFEN/CPB	+2.3	0.97	0.33	0.35	0.17	0.92	0.32

Table 2. Comparison of UNM solutions to IAEA 3-D benchmark problems

UNM Options	Δk_{eff} pcm	FA power density error, %		Node average fast flux error, %		Node average thermal flux error, %	
		$\varepsilon_{\max}^{a)}$	$\varepsilon_{rms}^{b)}$	$\varepsilon_{\max}^{a)}$	$\varepsilon_{rms}^{b)}$	$\varepsilon_{\max}^{a)}$	$\varepsilon_{rms}^{b)}$
NEM/QPA	-7.7	1.53	0.79	1.66	0.77	1.53	0.80
ANM/QPA	+4.6	1.50	0.54	0.62	0.28	1.51	0.53
ANM/ATL	+1.9	0.83	0.29	0.29	0.14	0.84	0.28
AFEN/MSS	-11.8	0.73	0.31	0.70	0.35	0.73	0.31
AFEN/CPB	+1.2	0.92	0.30	0.34	0.15	0.92	0.29

Table 3 Comparison of UNM Solutions to L336 C3 Problem

UNM Options	Δk_{eff} pcm	FA power density error, %		Node average fast flux error, %		Node average thermal flux error, %	
		$\varepsilon_{\max}^{a)}$	$\varepsilon_{rms}^{b)}$	$\varepsilon_{\max}^{a)}$	$\varepsilon_{rms}^{b)}$	$\varepsilon_{\max}^{a)}$	$\varepsilon_{rms}^{b)}$
NEM/QPA	-122.2	1.28	1.13	0.26	0.18	1.52	1.42
ANM/QPA	+20.3	0.23	0.21	0.02	0.02	0.28	0.26
ANM/ATL	+10.1	0.12	0.10	0.02	0.01	0.15	0.14
AFEN/MSS	+1.4	0.10	0.09	0.12	0.11	0.08	0.07
AFEN/CPB	+2.4	0.02	0.02	0.05	0.05	0.01	0.01

a) Maximum error

b) Root mean square error

The AFEN option is advantageous from the standpoint of accuracy, yet it takes more computational time than the TINM options because of extra computational efforts to determine the corner point fluxes either by the MSS or through the CPB equations. Tables 4 compare the CPU times of various UNM solutions to IAEA 3-D PWR problems on the octant symmetry. T_d denotes the CPU time spent solely for solving the UNM formulation of 2-G diffusion equations excluding input and output editing. As a matter of course, T_d depends on the convergence criterion and is measured by imposing relative flux convergence criterion of 10^{-7} for the conventional iteration scheme and relative residual convergence criterion of 10^{-7} for the nonlinear iteration scheme. As an additional convergence criterion for nonlinear iteration scheme, the convergence criterion of 10^{-5} is imposed for two correction factors. In terms of T_d, the AFEN options take the longest time among several nodal options. When the conventional iteration scheme is adopted, the AFEN/CPB option takes about twice the CPU time of the TINM option. Nonlinear nodal iterative schemes reduce the CPU time considerably. Their effectiveness is conspicuous particularly in the IAEA 3-D problem. From Table 4 we observe that the one-node nonlinear iteration scheme is very effective in reducing the CPU time of the conventional scheme. We also notice that the two-node nonlinear scheme is outperformed by the one-node scheme in the CPU time and the convergence of the solution – particularly in the IAEA 3-D solution by the AFEN option. To guarantee convergence of the IAEA 3-D solution, the two-node scheme requires adoption of an under-relaxation scheme in updating the transverse leakage coefficients. T and N_{out} in this case depend on the value of the relaxation parameter. $\omega = 0.5$ appears a reasonable choice for 1 N/FA IAEA 3-D calculation.

Table 4. Comparison of computational times for the UNM solutions to IAEA 3-D problem on the Alpha 21164 600MHz computer system (unit: seconds)

UNM options	Relaxation Parameter	Conventional Iteration Scheme [a]		Nonlinear Nodal Iteration Scheme [b]			
				One-node kernel		Two-node kernel	
		T_d	N_{out}	T_d	N_{out}	T_d	N_{out}
NEM	-	18.4	1211	1.37	12	1.67	13
ANM/QTL	-	21.1	1214	1.50	12	1.80	13
ANM/ATL	-	21.4	1214	1.53	12	1.90	13
AFEN/MSS	1.0	37.7	1235	2.21	12	N/C[c]	N/C[c]
	0.5	37.5	1232	2.14	11	6.20	42
	0.4	37.0	1232	2.25	12	4.57	29
	0.3	37.3	1232	2.83	15	5.20	34
AFEN/CPB	1.0	56.9	1252	3.09	14	N/C[c]	N/C[c]
	0.6	54.7	1248	2.60	13	10.7	65
	0.5	55.8	1248	2.70	12	6.11	35
	0.4	55.3	1248	2.71	13	6.27	37
	0.3	54.7	1248	3.39	15	6.40	39

a) Flux convergence criterion : 10^{-7}

b) Relative residual convergence criterion : 10^{-7}

c) Not converged

Finally, the UNM formulation of the AFEN method is more efficient in the computational speed than the original AFEN formulation. Figure 2 compares the maximum flux error reduction trends of the iterative solutions by the original AFEN and the UNM formulations for the quarter-core IAEA 2-D problem as a function of the number of the outer iterations (N_{out}). For the UNM calculation, the iterative solution procedure of the NEM is adopted without use of acceleration techniques. For the original AFEN calculation, the nodal coupling equations are put in a matrix eigenvalue problem for the eigenvalue k_{eff} and the eigenvector consisting of nodal unknowns; node average fluxes, nodal interface fluxes, and corner point fluxes. The flux error reduction trend of the original AFEN calculations depends on the number of inner iterations (N_{inner}) imposed on every outer iteration. Increasing N_{inner} from 1 to 2, 5, or 25 decreases N_{out} but requires more CPU time. When N_{inner}=1 is chosen, the original AFEN takes the least CPU time of 2.73 seconds. But this must be compared with the CPU time of 0.68 s taken by the UNM calculation. When one-node nonlinear UNM scheme is used, we observe that the number of outer iterations is reduced by an order of magnitude, and thus the CPU time for the solution to the IAEA 2-D problem is reduced to 0.14 second.

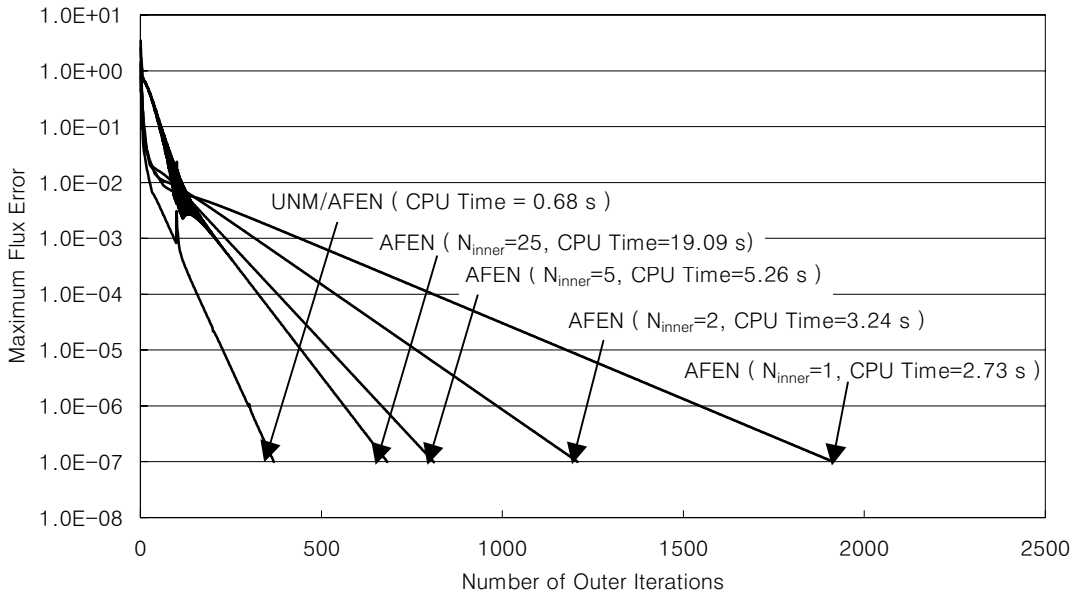

Figure 3. Maximum flux error reduction trends of the UNM and original AFEN method calculations with the number of outer iteration

5. CONCLUSIONS

From the standpoint of the AFEN method calculation, the UNM formulation has a minor deficiency in that equations determining transverse leakage expansion coefficients are poorly conditioned and thus need to take precaution against erroneous results. This appears a weakness of the UNM formulation that is absent in the original scheme. But we showed that this is easily overcome by adopting the under-relaxation scheme in updating

transverse leakage coefficients. We also showed that the UNM formulation is more effective in computational speed than the original AFEN formulation by comparison of flux error reduction trend with the number of iterations. In this conjunction, the one-node nonlinear iteration scheme introduced in this paper proves to be very effective for speedily convergent solution to our UNM formulation for the AFEN option. Besides the better computational efficiency, there are several other advantages of the UNM formulation for the AFEN method over the original AFEN formulation. It is simple to incorporate the AFEN option in the existing NEM code because all one has to do is add an extra subprogram for Eq. (12). One can utilize the well-established numerical schemes of NEM for speedy numerical solution of the AFEN option. Furthermore, the transient application is implemented in a straightforward manner, which we will demonstrate in our forthcoming paper.

REFERENCES

Argonne Code Center, Benchmark Problem Book, ANL-7416, Supplement 2, Argonne National Laboratory, June 1977.

Finnemann, H., Bennewitz F., Wagner, M. R., 1977. Interface Current Techniques for Multidimensional Reactor Calculations. *Atomkernenergie* **30**, 123-128.

Fischer, H. D., Finnemann, H., 1981. The Nodal Integration Method-A Diverse Solver for Neutron Diffusion Problems. *Atomkernenergie*, **39**, 229.

Fladmark, G. E., A method for the numerical solution of eigenvalue problems in diffusion theory," *Proc. Seminar on Numerical Reactor Calculations*, Vienna, 17-21 January 1972, pp497-507.

Hutt, P. et. al., 1991. The UK Core Performance Code Package. *Nuclear Energy J. British Nuclear Energy Society* **30**, 291.

Joo, H. G., Barber, D., Jiang, G., and Downar, T., 1998. PARCS : A Multi-Dimensional Two-Group Reactor Kinetics Code Based on the Nonlinear Analytic Nodal Method. PU/NE-98-26, Purdue University, September 1998.

Lee, H. C., Kim, C. H., 2000, Unified Nodal Formulation for Analytic Function Expansion Nodal Method Solution to Two-Group Diffusion Equations in Rectangular Geometry. *Trans. Am. Nucl. Soc.* **83**, 409-411.

Lee, H. C., Kim, C. H., 2000. A New Transverse Leakage Approximation for Improved Nodal Reactor Calculations. *Trans. Am. Nucl. Soc.* **83**, 411—414.

Lee, H. C., and Kim, C. H., 2001. Unified Formulation of NEM and ANM Solutions to Two Group Diffusion Equations. *Nucl. Sci. Eng*., to appear.

Lefebvre, J. C., Mondot, J., West, J. P. Benchmark Calculations of Power Distribution Within Assemblies, NEACRP-L-336, Organization of Economic Cooperation and Development 1977.

Moon, K. S., Cho, N. J., Noh, J. M., Hong, S. G., 1999. Acceleration of the Analytic Function Expansion Nodal Method by Two-factor Two-Node Nonlinear Iteration. *Nucl. Sci. Eng.* **132**, 194.

Noh, J. M., Cho, N. J., 1994. A New Approach of Analytic Basis Function Expansion to Neutron Diffusion Nodal Calculation. *Nucl. Sci. Eng*. **116**, 165.

Saad, Y., 1996. *Iterative Methods for Sparse Linear Systems,* PWR Publishing Company, Boston.

Shin, H. C., Kim, Y. H., Kim, Y. B., Bae, S. M., 1999. A Nonlinear Combination of CMFD (coarse-Mesh Finite Difference) and FMFD (Fine-Mesh Finite Difference) Methods. *Proc. KNS Spring Mtg*., Pohang, Korea, May 1999.

Smith, K. S., 1979. An Analytic Nodal Method for Solving the 2-Group, Multidimensional, Static and Transient Neutron Diffusion Equations, *Nucl. Eng. Thesis*, Dept. of Nucl. Eng., MIT.

Smith, K. S., 1983. Nodal Method Storage Reduction by Nonlinear Iteration. *Trans. Am. Nucl. Soc*. **44**, 265 (1983).

Turinsky P. et al., 1994. NESTLE : A Few-Group Neutron Diffusion Equation Solver. Electric Power Research Center, North Carolina State University, June 1994.