An AFEN Equivalent Hexagonal Nodal Method based on the Single-Node Nonlinear FDM Response Matrix

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1. Introduction

A hexagonal nodal method based on the analytic function expansion nodal (AFEN) method [2-7] is being developed and implemented into the CAPP code [1] to improve the computational efficiency of analyzing the prismatic high temperature gas cooled reactor cores. The AFEN version applied here is a refined one by adding the analytical basis functions combined with the transversedirection linear functions into the intranodal flux expansion [5]. The flux moments which are defined by the weighted average fluxes at the interface are used as nodal unknowns corresponding to the added basis functions. A linear function or a step function in parallel to the interface direction is used as a weighting function. On the other hand, the corner point fluxes are no longer used as nodal unknowns, since it is expected that sufficient accuracy can be achieved even without them. According to Reference 5, the refined AFEN method even without corner point fluxes provides much better accuracy than the original AFEN method.

In addition, the nodal method employs a response matrix method that uses the interface partial currents as nodal unknowns instead of the interface fluxes used in the original AFEN method. The response matrix method updates the outgoing partial currents of each node at each inner iteration step by imposing the incoming partial current boundary conditions on the interfaces of the node. Therefore, there is an advantage that the domain in calculation of the nodal unknowns and their coefficients matrixes can be confined within the node independently of its neighbor nodes.

Finally, the method adopts a computational acceleration method utilizing a two-factor coarse-mesh finite difference (CMFD) nonlinear iteration as in Reference 6. However, unlike Reference 6, which solves a two-node problem, here we solve a single-node problem and determine the interface non-linear correction factors. This can be justified it fits more to the concept of the response matrix which can be defined as the response (i.e., outgoing partial currents) of a single node to the input (i.e., incoming partial currents). Further evaluation is required for general reasoning that the stability of the overall calculation is reduced by utilizing the single node problem instead of the two node problem.

This is the initial step in implementing this method into the CAPP code. This paper reports the preliminary results of applying this method to a two-dimensional benchmark problem to evaluate its applicability to practical core analysis.

2. Methodology

2.1 Single-Node Nonlinear FDM Response Matrix

2.1.1 Nonlinear FDM Response Matrix

Reference 6 describes a nonlinear FDM iteration scheme in a rectangular node. Extending it to a hexagonal node begins by defining \widetilde{D}_{ρ}^{s} that is the nonlinear FDM correction factor at interface s of a node shown in Fig. 1 as follows:

$$J_g^s = -\frac{2D_g}{\sqrt{3}h}(\phi_g^s - \bar{\phi}_g) - \frac{2\widetilde{D}_g^s}{\sqrt{3}h}(\phi_g^s + \bar{\phi}_g)$$
(1)

where D_{σ} is the diffusion coefficient, ϕ_{σ}^{s} and J_{σ}^{s} the heterogeneous interface flux and the interface current, respectively, and $\overline{\phi}_{\sigma}$ is the node average flux.



Fig. 1. Interface s of a node

Noting that the heterogeneous interface flux and the interface current are given by

$$J_g^s = P_g^{out,s} - P_g^{in,s} \tag{2}$$

$$\phi_g^s = 2\left(\mathcal{P}_g^{out,s} + \mathcal{P}_g^{in,s}\right) \tag{3}$$

respectively. Here, $P_{a}^{out.s}$ and $P_{a}^{in.s}$ are the heterogeneous partial current going out from node n across interface s and the heterogeneous partial current coming in to node n, respectively.

Then, the outgoing partial current at interface s can be expressed in terms of the ingoing partial current at the same interface, as follows:

$$P_g^{out,s} = \frac{\sqrt{3}h - 4(D_g + \widetilde{D}_g^s)}{\sqrt{3}h + 4(D_g + \widetilde{D}_g^s)} P_g^{in,s} + \frac{2(D_g - \widetilde{D}_g^s)}{\sqrt{3}h + 4(D_g + \widetilde{D}_g^s)} \overline{\phi}_g \tag{4}$$

This is the so-called FDM response matrix, which provides an iterative process to solve the whole entire core eigenvalue problem assuming that the nonlinear FDM correction factor in this equation is known.

The correction factor is determined so that the solution of this nonlinear FDM is mathematically equivalent to the solution of the AFEN method. This is done by solving the single node problem by the AFEN method applying the procedure described in section 2.2. Once the AFEN solution is obtained, the correction factor is updated using the following equation:

$$\widetilde{D}_{g}^{s} = -\frac{\sqrt{3}hJ_{g}^{s} + 2D_{g}(\phi_{g}^{s} - \overline{\phi}_{g})}{2(\phi_{g}^{s} + \overline{\phi}_{g})}$$
(5)

In solving the single node problem by AFEN, the currents and the current moments at the six interfaces

are needed as the boundary conditions. Among them, the current boundary condition can be obtained from the partial currents converged by the nonlinear FDM iteration described above. However, an additional procedure is needed to obtain the current moments to provide the boundary conditions to the single node problem.

2.1.2 Interface Current Moment Scheme

We define the relationship between the current moment and the flux moment at the interface to be similar to the relationship between current and flux in Eq. (1).

$$j_{g}^{s} = -\frac{2D_{g}}{\sqrt{3h}}(\psi_{g}^{s} - \overline{\psi}_{g}) - \frac{2\widetilde{d}_{g}^{s}}{\sqrt{3h}}(\psi_{g}^{s} + \overline{\psi}_{g})$$
⁽⁶⁾

where $D_{Q_{g}}$ is again the diffusion coefficient and the others are the corresponding moment shadows to the relationship between flux and current.

Since the flux moment is defined only at the interface, it does not have its average value averaged over the node volume. For convenience, we define this value as the arithmetic mean of the flux moments at six interfaces.

$$\overline{\psi}_{\sigma} = \frac{1}{6} \sum_{s=1}^{6} \psi_{\sigma}^{s}$$
⁽⁷⁾

The correction factor for the current moment is also obtained from the AFEN solution of the single node problem utilizing the following equation:

$$\widetilde{d}_{g}^{s} = -\frac{\sqrt{3}h J_{g}^{s} + 2D_{g}(\psi_{g}^{s} - \overline{\psi}_{g})}{2(\psi_{g}^{s} + \overline{\psi}_{g})}$$

$$\tag{8}$$

If the partial current moment is defined to have a similar meaning to the partial current, it is also continuous across a interface and still satisfies the analogous relations to Eqs. (2) and (3).

$$j_a^s = p_a^{out,s} - p_a^{in,s} \tag{9}$$

$$\psi_a^s = 2\left(\rho_a^{out,s} + \rho_a^{in,s}\right) \tag{10}$$

Finally, an iterative process based on another response matrix is obtained to yield the interface partial current moments.

$$\rho_g^{out.s} = \frac{\sqrt{3}h - 4(D_g + \widetilde{d}_g^s)}{\sqrt{3}h + 4(D_g + \widetilde{d}_g^s)} \rho_g^{in.s} + \frac{2(D_g - \widetilde{d}_g^s)}{\sqrt{3}h + 4(D_g + \widetilde{d}_g^s)} \overline{\psi}_g$$
(11)

This iteration process involves a single inner iteration because it contains only the interface partial current moments as unknowns thanks to Eq. (7), Since this iteration is completely decoupled from the nonlinear FDM iteration given in Eq. (4), it can be done after the nonlinear FDM iteration is complete. This provides the additional advantage that the correction factors used in the two iterations can be stored sequentially in the same memory.

Alternatively to such an explicit scheme, an implicit nonlinear FDM schemes, where Eq. (1) and Eq. (6) are coupled with each other, can also be considered, for example:

$$J_g^s = -\frac{2D_g}{\sqrt{3}h}(\phi_g^s - \bar{\phi}_g) - \frac{2\widetilde{D}_g^s}{\sqrt{3}h}(\psi_g^s - \overline{\psi}_g)$$
(12)

$$J_{g}^{s} = -\frac{2D_{g}}{\sqrt{3}h}(\psi_{g}^{s} - \overline{\psi}_{g}) - \frac{2\widetilde{d}_{g}^{s}}{\sqrt{3}h}(\psi_{g}^{s} - \overline{\phi}_{g})$$
(13)

The numerical performance of this explicit scheme will be evaluated the following study.

2.2 AFEN Solution of Single-Node Problem [5]

2.2.1 Intranodal Flux Expansion

Solving the single node problem with interface current and current moment boundary conditions by the AFEN methods starts from expending the intranodal flux distribution into the analytic basis functions with and without transverse-direction linear functions.

$$\boldsymbol{\phi}(x, y) = \boldsymbol{\phi}(x, y) + \boldsymbol{\phi}(u, v) + \boldsymbol{\phi}(\mathcal{D}, q)$$
(14)

where

$$\boldsymbol{\varphi}(x, y) = \sinh\left(\sqrt{\mathbf{\Lambda}}x\right)\left(\mathbf{A}_{0}^{x} + \mathbf{A}_{1}^{x}y\right) + \cosh\left(\sqrt{\mathbf{\Lambda}}x\right)\left(\mathbf{B}_{0}^{x} + \mathbf{B}_{1}^{x}y\right)$$
(15)
$$\mathbf{\Lambda} = \mathbf{D}^{-1}\boldsymbol{\Sigma}$$
(16)

and **D** and **\Sigma** are the diffusion coefficient and crosssection matrixes, respectively. Here, (x, y), (u,v) and (p,q) are the three coordinates in Fig. 2 introduced for convenience.



Fig. 2. Coordinate systems and Nodal Unkowns

Note that this flux expansion has twelve terms with one coefficient each and all of them completely satisfy the diffusion equation for the node. Of course, both the basis functions and the coefficients of this expansion are square matrices with the number of energy groups as its order. However, thanks to the matrix function theory, they can be treated like scalar as long as they are functions of Λ .[8,9]

The average flux of the node is defined from this flux expansion as follows.

$$\overline{\mathbf{\phi}} = \frac{8\sqrt{3}}{9h^2} \int_0^{\frac{\sqrt{3}}{2}h} \int_0^{-\frac{\sqrt{3}}{3}x+h} \mathbf{\phi}(x, y) \, dy \, dx \quad . \tag{17}$$

The interface fluxes and the flux moments e.g., at the x1 interface are respectively defined by

$$\phi_1^x = \frac{1}{h} \int_{-\frac{h}{2}}^{\frac{h}{2}} \phi(\frac{\sqrt{3}}{2}h, y) dy$$
(18)

$$\Psi_{1}^{x} = \frac{1}{h} \int_{-\frac{h}{2}}^{\frac{h}{2}} w(y) \phi(\frac{\sqrt{3}}{2}h, y) dy$$
(19)

respectively. Here, w(y) is the weighting two types of w(y), i.e., the step function and the linear function of y are used as the weighting function.

$$w(y) = \begin{cases} -1 & when \ y < 0 \\ 1 & when \ y \ge 0 \end{cases} \quad \text{and} \quad w(y) = y \,. \tag{20}$$

If the step function is used, it is equivalent to the case where an interface is cut in half and the continuous condition of flux and current is applied for each half of the interface.

Strictly speaking, when applying equivalence theory, the interface fluxes and moments in Fig. 2 are different from those for the nonlinear FDM scheme shown in Fig. 1: The former are homogeneous ones and the latter are heterogeneous ones. However, for simplicity, we treat these two as the same kind here. In implementing, of course, the discontinuity factors were involved.

Further, the interface current and the current moment at the example interface are consistently defined by

$$\mathbf{J}_{x1}^{out} = -\frac{\mathbf{D}}{\hbar} \int_{-\frac{\hbar}{2}}^{\frac{\hbar}{2}} \frac{\partial}{\partial x} \mathbf{\phi}(x, y) dy \bigg|_{x = \frac{\sqrt{3}}{2}\hbar}$$
(21)

$$\mathbf{j}_{x1}^{out} = -\frac{\mathbf{D}}{h} \int_{-\frac{h}{2}}^{\frac{h}{2}} w(y) \frac{\partial}{\partial x} \mathbf{\phi}(x, y) dy \bigg|_{x = \frac{\sqrt{3}}{2}h}$$
(22)

2.2.2 AFEN Solution of Single-Node Problem

Solving the single node problem in Fig. 2 to obtain the intranodal flux distribution means expressing 12 coefficients of the flux expansion Eq. (14) in terms of 6 interface currents and 6 interface current moments. This problem seems to involve inversing a 12x12 matrix. However, the decoupling transformation of Reference 5 simplifies it to a problem of inversing several smaller matrixes.

This transformation transforms both the flux expansion coefficients and the nodal unknowns. First, the nodal unknowns are transformed into the even and the odd forms e,g., in the x-direction:

$$\boldsymbol{\omega}_{e}^{x} = \frac{\boldsymbol{\varphi}_{0}^{x} + \boldsymbol{\varphi}_{1}^{x}}{2} - \overline{\boldsymbol{\varphi}}, \quad \boldsymbol{\omega}_{0}^{x} = \frac{\boldsymbol{\varphi}_{0}^{x} - \boldsymbol{\varphi}_{1}^{x}}{2}$$
(23)

$$\boldsymbol{\sigma}_{e}^{x} = \frac{\boldsymbol{\Psi}_{0}^{x} + \boldsymbol{\Psi}_{1}^{x}}{2}, \qquad \boldsymbol{\sigma}_{o}^{x} = \frac{\boldsymbol{\Psi}_{0}^{x} - \boldsymbol{\Psi}_{1}^{x}}{2}$$
(24)

Applying symmetric thinking, the even and the odd forms of the interface currents and current moments are defined as follows:

$$\mathbf{\eta}_{e}^{x} = \frac{\mathbf{J}_{x1}^{'n} + \mathbf{J}_{x0}^{'n}}{2}, \quad \mathbf{\eta}_{o}^{x} = \frac{\mathbf{J}_{x1}^{'n} - \mathbf{J}_{x0}^{'n}}{2}$$
(25)

$$\mathbf{\varsigma}_{e}^{x} = \frac{\mathbf{j}_{x1}^{'n} + \mathbf{j}_{x0}^{'n}}{2}, \quad \mathbf{\varsigma}_{o}^{x} = \frac{\mathbf{j}_{x1}^{'n} - \mathbf{j}_{x0}^{'n}}{2}$$
 (26)

,respectively.

Now, the coefficients of the expansion flux and the nodal unknowns are transformed once again as shown below.

$$\mathbf{C}_{k\theta} = \frac{\mathbf{C}_{k}^{\times} + \mathbf{C}_{k}^{u} + \mathbf{C}_{k}^{p}}{3}, \quad \mathbf{C}_{k\varepsilon} = \frac{2\mathbf{C}_{k}^{\times} - \mathbf{C}_{k}^{p} - \mathbf{C}_{k}^{p}}{3}, \quad \mathbf{C}_{k\chi} = \frac{\mathbf{C}_{k}^{u} - \mathbf{C}_{k}^{p}}{3}$$
(27)

$$\boldsymbol{\omega}_{s\theta} = \frac{\boldsymbol{\omega}_{s}^{x} + \boldsymbol{\omega}_{s}^{\mu} + \boldsymbol{\omega}_{s}^{p}}{3}, \quad \boldsymbol{\omega}_{s\varepsilon} = \frac{2\boldsymbol{\omega}_{s}^{x} - \boldsymbol{\omega}_{s}^{\mu} - \boldsymbol{\omega}_{s}^{p}}{3}, \quad \boldsymbol{\omega}_{s\chi} = \frac{\boldsymbol{\omega}_{s}^{\mu} - \boldsymbol{\omega}_{s}^{p}}{3}$$
(28)

$$\boldsymbol{\sigma}_{s\theta} = \frac{\boldsymbol{\sigma}_{s}^{x} + \boldsymbol{\sigma}_{s}^{u} + \boldsymbol{\sigma}_{s}^{p}}{3}, \quad \boldsymbol{\sigma}_{s\varepsilon} = \frac{2\boldsymbol{\sigma}_{s}^{x} - \boldsymbol{\sigma}_{s}^{u} - \boldsymbol{\sigma}_{s}^{p}}{3}, \quad \boldsymbol{\sigma}_{s\chi} = \frac{\boldsymbol{\sigma}_{s}^{u} - \boldsymbol{\sigma}_{s}^{p}}{3}$$
(29)

where coefficient letter C is A or B, interface index k is 0 or 1 and even-odd index s is e or o.

Expressing the transformed unknowns in terms of the transformed expansion coefficients, we can realize that the original 12x12 matrix equation is decoupled with four 2x2 matrix equations and four scalar equations. In particular, two of the four 2x2 matrixes are in the relationship of similarity transformation to the other two. Therefore, solving a single-node problem simply involves finding the inverses of two 2x2 matrixes and four scalars, for example:

$$\begin{bmatrix} \boldsymbol{\omega}_{\circ \boldsymbol{\chi}} \\ \boldsymbol{\sigma}_{\circ \boldsymbol{\varepsilon}} \end{bmatrix} = \mathsf{T} \begin{bmatrix} \mathsf{A}_{\circ \boldsymbol{\chi}} \\ \mathsf{B}_{1 \boldsymbol{\varepsilon}} \end{bmatrix} \text{ and } \begin{bmatrix} \boldsymbol{\eta}_{\circ \boldsymbol{\chi}} \\ \boldsymbol{\varsigma}_{\circ \boldsymbol{\varepsilon}} \end{bmatrix} = \mathsf{M} \begin{bmatrix} \mathsf{A}_{0 \boldsymbol{\chi}} \\ \mathsf{B}_{1 \boldsymbol{\varepsilon}} \end{bmatrix}$$
(30)

where M and T are $2x^2$ matrixes with elements of Λ matrix functions.

By eliminating the coefficient vector, the interface fluxes and flux moments can be expressed in terms of the interface currents and current moments, which are boundary conditions e.g., as follows:

$$\begin{bmatrix} \mathbf{\omega}_{o_{\chi}} \\ \mathbf{\sigma}_{e_{\varepsilon}} \end{bmatrix} = \mathbf{T} \mathbf{M}^{-1} \begin{bmatrix} \mathbf{\eta}_{o_{\chi}} \\ \mathbf{\varsigma}_{e_{\varepsilon}} \end{bmatrix}$$
(31)

As is known, the inverse of M is singular when one of the eigenvalues of the crosssection matrix is very small. This singularity is removed in the manner described in Reference 5.

Since all the transformations so far are linear, their inverse transformations are also linear. Therefore, an original nodal unknown as e.g., in Eq. (18) is expressed as a linear combination of transformed unknowns as e.g., in Eq. (28), and vice versa.

Once the interface fluxes and flux moments are calculated from the interface currents and current moments resulting from the nonlinear FDM iteration with Eq. (4), the nonlinear FDM correction factors to be used in the nonlinear FDM iteration are calculated in turn using Eqs. (5) and (8).

2.2.3 RGB Sweeping Scheme

As described above, when the response matrix method is applied, both the single-node AFEN calculation and the nonlinear FDM response calculation are performed only within a single node regardless of neighboring nodes. Therefore, these calculations are carried out by sequentially moving from one node to another. In this case, it is advantageous to sweep the nodes by dividing them into red (R), green (G), and blue (B) nodes as shown in Fig. 3, like checkerboard sweeping for a rectangular node core.



Fig. 3. RGB sweeping scheme

First of all, this kind of iteration schemes is known to be good in convergence and stability due to geometrical balance. In addition, the memory required is saved by storing inputs of the response calculation, i.e., incoming partial currents and outputs, i.e., outgoing partial currents in the same storage. This is because the outgoing partial currents resulting from previous two other types of node calculations automatically become incoming partial currents for the third kind of node calculations.

3. Numerical Results and Discussion

In order to verify the nodal method developed in this study, we solved several benchmark problems including a mini core problem which was derived from VVER-440 benchmark problem [5]. However, the results are unsatisfactory in terms of acceleration performance. In some cases, it took more computation time than original AFEN, or even failed to converge. The cause of convergence degradation may be that it is based on a one-node problem that is less stable than a two-node problem. Or it may be due to the model of the interface partial current moment given by Eq. (11).

The results of the mini core benchmark is shown in Fig.4 to verify that the proposed nonlinear FDM-based response matrix method is mathematically equivalent to the original refined AFEN. As shown in the figure, the two results are de facto identical within the number of meaningful digits of main output. It is not appropriate to present the computation time for the mini core at this stage. The acceleration performance of the proposed scheme will be evaluated comprehensively after significant efforts are made to improve convergence, such as using a two-node problem instead of the one-node problem or using the implicit model of the partial current moment presented in Eq. (12) and (13).



Fig. 4. Results of the mini core problem (1/6 core)

4. Conclusions

In order to improve efficiency of the CAPP code in the analysis of the HTGR core, a nonlinear FDM-based response matrix method in the hexagonal geometry has been developed in a manner that it is equivalent to the refined AFEN method. In the nodal method, the corner point fluxes are no longer nodal unknowns, but the flux moments which are defined by the weighted average fluxes at the interface take the role of nodal unknowns.

In addition, the method adopts a two-factor coarsemesh finite difference (CMFD) nonlinear iteration as in Reference 6. It solves the single node problem by the AFEN method to determine the interface nonlinearity correction factors instead of the two-node problem as utilized in Reference 6.

This method was tested against several benchmark problems and verified that it could provide the equivalent results to the original refined AFEN method. However it failed to show computational acceleration performance due to possible defects in the one-node problem or the partial current moment model. This is the initial step of porting this method to the CAPP code. The method will be improved with efforts such as adopting a two-node problem instead of the one-node problem or using the implicit model of the partial current moment.

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