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Source Expansion Nodal Method for Hexagonal Geometry Applications

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1. Introduction

With the continued need for fast reactor and high temperature reactor analysis, there has been steady interest in hexagonal geometry nodal codes. The Analytic Function Expansion Nodal method (AFEN)[1] and the Triangle-based Polynomial Expansion method (TPEN)[2] are one of the nodal methods which do not involve transverse integration and directly find the two-dimensional(2D) intra-nodal flux distributions. The AFEN method which yields quite accurate solutions, however, is not efficient in multi-group problems which are encountered in fast reactor analyses, whereas the TPEN method is less accurate for large node problems encountered in high temperature reactor analyses. On the other hand, the source expansion nodal method (SENM)[3] was developed as a semi-analytic nodal method that renders sufficient accuracy and ease of multi-group applications. But it was limited to Cartesian geometry and employed transverse integration. The SENM type 2D expansion was tried for pin power reconstruction in rectangular fuels.[4] In the work here, the SENM with 2D source expansion is extended to hexagonal geometry applications. In the following, the SENMH, the hexagon version of SENM, is derived and examined for a set of simple 2D and 3D core problems that involve heavily rodded configurations.

2. Semi-analytic solution with 2D source expansion

In the source expansion nodal method, the analytic solution is obtained for the 2D neutron diffusion equation after moving all the source terms to the right hand side (RHS) and then approximating the source distribution by a polynomial. The analytic solution in this case consists of the exponential homogeneous solution and the polynomial particular solution. Thus the resulting source has the exponential terms as well as the polynomial terms. The exponential function is expanded into a polynomial in the next iteration step and this expansion of the source distribution is the main idea of the SENM. This source expansion is possible by the group decoupling scheme which treats the source distribution as known from the previous iterative solution. The analytic solution can be easily obtained for each group with the decoupling scheme. Because of the polynomial expansion with a finite number of terms, however, the SENM solution can be less accurate than the fully analytic solution. The accuracy of the semi-analytic solution would increase as the number of terms in the source polynomial increases.

By the way, the homogeneous solution of the 2D neutron diffusion equation is the solution of the Helmholtz equation which can be expressed in terms of infinite number of combination of x and y directional buckling values. With a finite number of boundary conditions, however, specific angles need to be determined. Cho and Noh[1] chose 12 angles which are 30°, 60°, 90°, and the other angles with 30° apart. The same homogeneous solution form will be used in the following derivation of the 2D SENM solution for hexagons.

2.1 Two-dimensional SENM for Hexagons

After integrating the 3D neutron diffusion equation axially over a plane of thickness, h_z, the following 2D balance equation is obtained for each group with the source terms moved to the right hand side:

$$\begin{aligned}&-D_g\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)\phi_g(x,y)+\Sigma_{rg}\phi_g(x,y)\\&=\frac{1}{k}\chi_g\sum_{g'}\nu\Sigma_{fg'}\phi_{g'}(x,y)+\sum_{g'\neq g}\Sigma_{g'g}\phi_{g'}(x,y)-L_{gz}(x,y)\end{aligned} \quad (1)$$

where the axial transverse leakage is defined as $L_{gz}(\xi,\eta)=\left(J_{gz}^r(\xi,\eta)-J_{gz}^l(\xi,\eta)\right)/h_z$ in term of the currents at the top and bottom surfaces of the plane; and k is the multiplication factor. The entire right hand side (RHS) term can be iteratively updated and approximated by a polynomial of two spatial coordinate variables. With such a polynomial approximation, the solution of Eq. (1) would be obtained in a straightforward manner.

Since it is advantageous to use the Legendre polynomial for the polynomial approximation owing to its orthogonal property, we normalize the independent variable such that it varies from -1.0 to 1.0 in the node. This leads to the following equation with the group index g omitted:

$$-\frac{4D_g}{h^2}\left(\frac{\partial^2}{\partial\xi^2}+\frac{\partial^2}{\partial\eta^2}\right)\phi_g(\xi,\eta)+\Sigma_{rg}\phi_g(\xi,\eta)=Q(\xi,\eta) \quad (2)$$

where h is the hexagon pitch; $\xi=2x/h$, $\eta=2y/h$; and $Q(\xi,\eta)$ represents the distribution of the entire sources. As the polynomial approximation to the source distribution, we use a quartic polynomial given in terms of the products of Legendre polynomials:

$$Q(\xi,\eta)=\sum_{i=0}^{4}\sum_{j=0}^{4}q_{i,j}P_i(\xi)P_j(\eta)\,,\ (i+j\le 4) \quad (3)$$

where $P_i(\xi)$ is the $i-$th order Legendre polynomial. Note that this 15 term polynomial contains fourth order cross-terms such as $P_1(\xi)P_3(\eta)$ and $P_2(\xi)P_2(\eta)$ representing a maximum quartic variation in each direction. In the following, it will be assumed that the source term coefficients are known and so are the 12 boundary conditions for each group flux.

The particular solution of Eq. (2) can be easily obtained by assuming the same polynomial form as the source, Eq. (3). Specifically, the coefficients, c_{ij}, of the polynomial particular solution, $\phi^P(\xi,\eta)$, can be determined by the method of undetermined coefficient. The first two of them are obtained as:

$$c_{0,0} = \frac{48D^2\left(35\left(q_{0,4}+q_{4,0}\right)+6q_{2,2}\right)}{h^4\Sigma_r^3} + \frac{4D\left(3\left(q_{0,2}+q_{2,0}\right)+10\left(q_{0,4}+q_{4,0}\right)\right)}{h^2\Sigma_r^2} + \frac{q_{0,0}}{\Sigma_r} \tag{4}$$

On the other hand, the homogeneous equation of Eq. (2) can be rewritten as follows by dividing by $4D/h^2$:

$$\left(\frac{\partial^2}{\partial\xi^2}+\frac{\partial^2}{\partial\eta^2}\right)\phi_g\left(\xi,\eta\right) = B_t^2\phi\left(\xi,\eta\right) \tag{5}$$

where the dimensionless buckling is defined as:

$$B_t^2 = \frac{h^2\Sigma_r}{4D} = \frac{h^2}{4L^2} \tag{6}$$

with L being the diffusion length. Eq. (5) can be solved by separation of variables after splitting the total buckling as follows:

$$B_t^2 = B_{t,\xi}^2 + B_{t,\eta}^2 \tag{7}$$

where $B_{t,\xi} = B_t\cos\theta$ and $B_{t,\eta} = B_t\sin\theta$. Among infinitely many combinations for the splitting, we choose only twelve pairs corresponding to the following angles:

$$\theta_k = \frac{\pi}{6}k, \quad k = 0...11 \tag{8}$$

which would require only twelve boundary conditions as was done by Böer and Finnemann[5]. Fig. 1. shows how the boundary condition is applied in the hexagonal node.

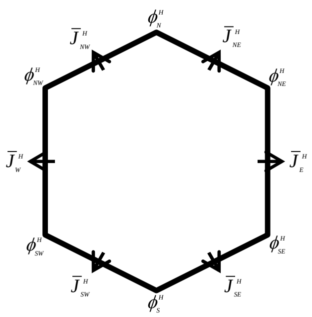

Fig. 1. Boundary conditions for hexagonal geometry.

This leads to the following form of the homogeneous equation:

$$\phi^H\left(\xi,\eta\right) = \sum_{k=0}^{11}\hat{a}_k e^{B_t\left(\xi\cos\theta_k+\eta\sin\theta_k\right)} \tag{9}$$

which can be rewritten in terms of *sinh* and *cosh* as:

$$\begin{aligned}
\phi_H\left(\xi,\eta\right) &= a_1\sinh\left(B_t\xi\right)+a_2\cosh\left(B_t\xi\right)+a_3\sinh\left(B_t\eta\right)+a_4\cosh\left(B_t\eta\right) \\
&+a_5\sinh\left(\frac{\sqrt{3}B_t\xi}{2}\right)\cosh\left(\frac{B_t\eta}{2}\right)+a_6\sinh\left(\frac{\sqrt{3}B_t\xi}{2}\right)\sinh\left(\frac{B_t\eta}{2}\right) \\
&+a_7\cosh\left(\frac{\sqrt{3}B_t\xi}{2}\right)\sinh\left(\frac{B_t\eta}{2}\right)+a_8\cosh\left(\frac{\sqrt{3}B_t\xi}{2}\right)\cosh\left(\frac{B_t\eta}{2}\right) \\
&+a_9\sinh\left(\frac{\sqrt{3}B_t\eta}{2}\right)\cosh\left(\frac{B_t\xi}{2}\right)+a_{10}\sinh\left(\frac{\sqrt{3}B_t\eta}{2}\right)\sinh\left(\frac{B_t\xi}{2}\right) \\
&+a_{11}\cosh\left(\frac{\sqrt{3}B_t\eta}{2}\right)\sinh\left(\frac{B_t\xi}{2}\right)+a_{12}\cosh\left(\frac{\sqrt{3}B_t\eta}{2}\right)\cosh\left(\frac{B_t\xi}{2}\right)
\end{aligned} \tag{10}$$

In deriving the twelve homogeneous solution coefficients, it is easy to convert the boundary condition to be applied only to the homogeneous solution by subtracting the particular solution part from the actual boundary condition. This is because the particular solution is always determined uniquely once the source polynomial is specified. The applied form of 6 boundary conditions to the homogeneous and particular solution is following as summation form. Eq. (11) represents only the 3 boundary conditions northern part of hexagonal geometry:

$$\begin{aligned}
\phi_{NE}^H &= \phi_{NE} - \phi_{NE}^P = \phi\left(\frac{\sqrt{3}}{2},\frac{1}{2}\right) - \sum_{i=0}^{4}\sum_{j=0}^{4}c_{i,j}P_i\left(\frac{\sqrt{3}}{2}\right)P_j\left(\frac{1}{2}\right), \\
\phi_N^H &= \phi_N - \phi_N^P = \phi(1,0) - \sum_{i=0}^{4}\sum_{j=0}^{4}c_{i,j}P_i(1)P_j(0), \\
\phi_{NW}^H &= \phi_{NW} - \phi_{NW}^P = \phi\left(-\frac{\sqrt{3}}{2},\frac{1}{2}\right) - \sum_{i=0}^{4}\sum_{j=0}^{4}c_{i,j}P_i\left(-\frac{\sqrt{3}}{2}\right)P_j\left(\frac{1}{2}\right),
\end{aligned} \tag{11}$$

For instance, the homogenous part of the flux at the north corner $(\xi = 0, \eta = 1)$ is obtained as:

$$\begin{aligned}
\phi_N^H &= \phi_N - \phi_N^P \\
&= \phi_N - c_{0,0} - c_{0,1} - c_{0,2} - c_{0,3} - c_{0,4} \quad . \\
&+ \frac{c_{2,0}}{2} + \frac{c_{2,1}}{2} + \frac{c_{2,2}}{2} + \frac{3c_{4,0}}{8}
\end{aligned} \tag{12}$$

while the surface average current at the surface is given as an integral form like below. Eq. (14) represents only the 3 eastern part of surface average current boundary condition as:

$$\begin{aligned}
\bar{J}_E^H &= \bar{J}_W - \int_{-1/2}^{1/2} J_x^P\left[1,\eta\right]d\eta \\
\bar{J}_{NE}^H &= \bar{J}_{NE} - \int_0^{\sqrt{3}/2} J_u^P\left[\xi,-\frac{\xi}{\sqrt{3}}+1\right]d\xi,\ \eta = -\frac{\xi}{\sqrt{3}}+1 \quad . \\
\bar{J}_{SE}^H &= \bar{J}_{SE} - \int_0^{\sqrt{3}/2} J_{-v}^P\left[\xi,\frac{\xi}{\sqrt{3}}-1\right]d\xi,\ \eta = \frac{\xi}{\sqrt{3}}-1
\end{aligned} \tag{13}$$

The homogeneous part of the corner fluxes and the surface average currents are obtained as above.

Using these boundary conditions, the coefficients of homogeneous solutions are determined. The coefficients given in Eqs. (4) and (10) for the particular and homogeneous solutions define the final solution:

$$\phi(\xi,\eta) = \phi_H(\xi,\eta) + \phi_P(\xi,\eta). \qquad (14)$$

2.2 Source Expansion

In the above derivation, it was assumed that the source distribution is known and it is described by a quartic polynomial of two unknowns. With the new 2D solution flux solution available, the primary source distribution which consists of the fission and scattering sources should be updated for the use in the next step of the iterative solution sequence. Since the 2D flux distribution for each group contains the exponential function components as well as the polynomial function components whereas the source is to be approximated by only a polynomial function, it is necessary to obtain first the 2D quartic polynomial approximation of the flux distribution for each group. Then the source term coefficients can be obtained by multiplying the flux coefficients by the proper cross-section and then by summing over the groups.

The method of approximation is the least square fitting which corresponds to the orthogonal expansion of an analytic function in terms of the Legendre function. The expansion coefficients can be obtained as $p_{i,j}$:

$$p_{i,j} = \frac{\int_{-1}^{1}\int_{-1}^{1}\phi(\xi,\eta)P_i(\xi)P_j(\eta)d\xi d\eta}{\int_{-1}^{1}\int_{-1}^{1}P_i(\xi)P_j(\eta)d\xi d\eta} \quad i+j \le 4 \qquad (15)$$

Using the coefficients obtained by Eq. (15), the flux and source term including fission and scattering sources are determined as

$$\phi_{\perp}(\xi,\eta) = \sum_{i=0}^{4}\sum_{j=0}^{4} p_{i,j}P_i(\xi,\eta)P_j(\xi,\eta) \ , \ i+j \le 4 \qquad (16)$$

$$q_{i,j}^{g} = \frac{\chi_g}{k_{eff}}\sum_{g'}\nu\Sigma_{fg'}c_{i,j}^{g'} + \sum_{g'\neq g}\Sigma_{g'g}c_{i,j}^{g'} - l_{i,j}^{g}. \qquad (17)$$

2.3 Determination of Corner Flux

In order to determine the twelve coefficients of the homogeneous solution, the six values of the corner fluxes should be specified. In the previous work [4] for rectangles, so called the corner point balance (CPB) condition was used that requires the sum of the four values of the differences in the net current obtained around a corner point to be zero.

Consider now a corner surrounded by 3 nodes as shown in Fig. 2 for hexagons. From the 2D flux solution of each node, 3 directional net current at the corner become available. Firstly the partial currents are defined as:

$$J_{c,k}^{\mp} = \frac{1}{4}\phi_{c,k} \mp \frac{1}{2}e_{c,k}J_{c,k} \qquad (18)$$

where k is the index of corner points. $J_{c,1}$ is the corner position at the upper right and counter clock-wisely the corner points are numbered. For the 3 nodes, there are 3 sets of directional currents. And using the definition of partial currents, the CPB can be written as [6]:

$$\left(J_{c,1}^{+,1} - J_{c,1}^{-,1}\right) + \left(J_{c,3}^{+,2} - J_{c,3}^{-,2}\right) + \left(J_{c,5}^{+,3} - J_{c,5}^{-,3}\right) = 0 \qquad (19)$$

In principle, the 3 directional currents must be the same. But since no continuity condition is imposed, there can be difference in the net currents. Using those net currents difference, the new corner flux can be obtained by taking the average of them as Eq. (20):

$$\phi_c^{new} = \frac{2}{3}\left\{\left(J_{c,1}^{+,1} + J_{c,1}^{-,1}\right) + \left(J_{c,3}^{+,2} + J_{c,3}^{-,2}\right) + \left(J_{c,5}^{+,3} + J_{c,5}^{-,3}\right)\right\}. \qquad (20)$$

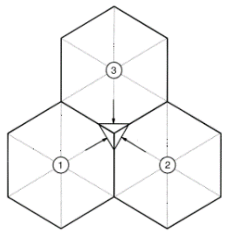

Fig. 2. Corner point balance model.

3. Assessment

A series of the benchmark problems with hexagonal nodes have been solved with the TPEN module of the RENUS code [2]. In order to verify the SENMH method, the same benchmark problems are used. One of the benchmark problems is for a small hexagonal core whose assembly pitch is about 7 cm. In addition, various control rod inserted problems are solved to examine the solution error with respect to the extent of control rod insertion. For the comparison, the results of the McCARD[7] multi-group Monte Carlo calculations are used as the reference.

At first, a set of minicore problems consisting of single assembly composition was solved to compare with the result of TPEN. Secondly the control rod inserted problems solved with 4 types of control rod insertion configurations.

3.1 Mini Core Problems

The control rod inserted problems for the 2D core shown in Fig. 3 involves very steep flux gradients. There are 4 conditions of control rod insertion.

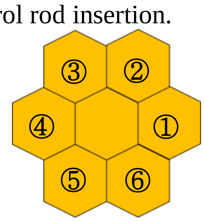

Fig. 3. Mini core configuration and control rod positions.

In Table I, the first column shows the control rod inser-ted position. It is clearly noted in this table that the error between reference data and other data is gradually increased for the TPEN solver. In the SENMH case, however, the increase in error is much less than TPEN.

Table I. Results for Control Rod Inserted Problem

Position	McCARD	SENMH($\Delta\rho$,pcm)	TPEN($\Delta\rho$,pcm)
ARO	1.52143	1.52110(14)	1.52111(14)
1	1.37597	1.37532(34)	1.37756(84)
1,3,5	1.16218	1.16132(63)	1.16587(272)
ARI	0.98247	0.98152(99)	0.98786(555)

3.2 Large Core Problems

The large 3D core problems shown in Fig. 4 also involves control rod insertion as well as unrodded configuration.

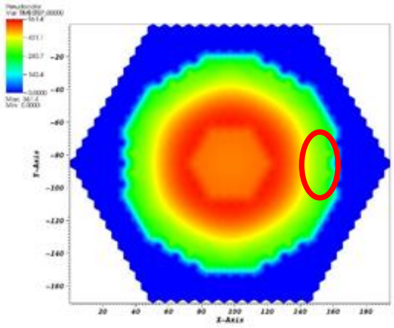

Fig. 4. Model core power distribution and removed control rod position (circle).

The results for the 3-D core problem given in Table II show the same tendency for the control rod inserted problem as in Table I. The error of TPEN that amounts 400 pcm is too large for this asymmetrically rodded problem.

Table II. Results for 3D Core Problem

Position	McCARD	SENMH($\Delta\rho$,pcm)	TPEN($\Delta\rho$,pcm)
ARO	1.02996	1.03028(30)	1.03026(28)
CR Inserted	0.99452	0.99562 (111)	0.99871(422)

4. Conclusion

An alternative method for the hexagonal geometry nodal solution has been established. Using the concept of source expansion in a hexagon, the SENMH method was derived such that the homogeneous solution coefficients are determined by 6 surface averaged currents and 6 corner fluxes while the particular solution coefficients are determined by a 15 term quartic polynomial coefficients for the source term. The corner point fluxes are determined by imposing the corner point balance condition. With the two solutions, the updated source is constructed using the Legendre expansion concept. This procedure is iteratively performed until convergence is reached.

The accuracy of SENMH was verified for a set of simple minicore and 3D problems having different control rod insertion configurations. The superior accuracy of SENMH was observed for the control rod inserted problems which involve steep flux gradients. The result showed much better accuracy than the TPEN method in that the reactivity error can be decreased by more than 400 pcm for the very heavily rodded case. It was thus concluded that SENMH can replace TPEN with the merit of superior accuracy while retaining the advantage of multi-group applications.

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