DEVELOPMENT OF A POLYNOMIAL NODAL MODEL FOR THE MULTIGROUP DIFFUSION EQUATION IN 2-D

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ABSTRACT

A nodal model which uses Legendre polynomials as the expansion functions is developed for the 2-D multigroup diffusion equation. The coefficients of the unknown polynomials are calculated from a set of linear equations. These equations are obtained as a result of applying the least-squares method and the use of the interface conditions. The interface conditions are the integrated 1-D partial currents. The IAEA-2D benchmark problem is used to check the accuracy of the nodal model. The results are compared with finite-difference and Green's Function nodal method solutions of the 2-D diffusion equation and shows that the model compared favorably.

1. INTRODUCTION

Three papers have described a particular type of nodal model for the solution of the one, two and three-dimensional multigroup diffusion equation (Rohach 1986a, 1986b, and 1987). In the nodal models described by Rohach, the fourth-order Legendre polynomials are used as the trial functions while average neutron fluxes and currents are used at the nodal interfaces. The method of solution used in the aforementioned nodal models is based on an iterative process in which the unknown polynomial coefficients are evaluated from a set of linear equations. These equations are obtained from the least-squares minimization of the polynomial expansion residuals and the interface conditions. Once the polynomial coefficients are found in a given iteration, new interface conditions and the eigenvalue are calculated. The iteration process is then continued until a given convergence criterion is satisfied.

In the nodal model reported upon here, the neutron flux is expanded as Legendre polynomials in both of the spatial variables. The model is not limited to the fourth-order expansion as was the case with the preceding papers. In addition, the average one dimensional partial currents are extended to the two dimensional case and used as the interface conditions.

2. 2-D DIFFUSION THEORY NODAL MODEL

The 2-D multigroup diffusion equation with constant neutronic parameters is given by Duderstadt and Hamilton (1976) as:

$$D^g \left[\frac{\partial^2 f^g(x,y)}{\partial x^2} + \frac{\partial^2 f^g(x,y)}{\partial y^2} \right] - \Sigma_t^g f^g(x,y) + \sum_{h=1}^{G} a^{gh} f^h(x,y) = 0, \qquad (1)$$

where

$$\Sigma_t^g = \Sigma_a^g + \sum_{h=1}^{G} \Sigma_s^{hg},$$

and

$$a^{gh} = \frac{1}{l} c^g n \Sigma_f^h + \Sigma_s^{gh}, \qquad (2)$$

The development of the nodal model begins by dividing the two-dimensional region into a number of nodes. Each node has its own coordinate system located at the center of the node as shown in Fig.1.

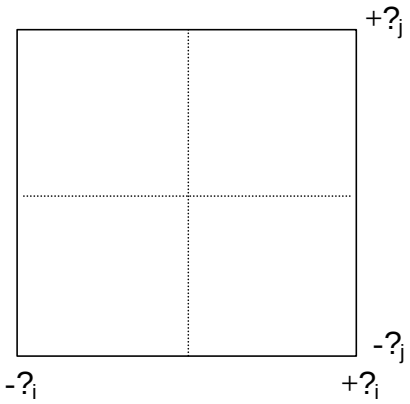

Fig.1 node(i,j)

Due to the orthogonality of the Legendre polynomials in the range of -1 and +1, the development of the equations will be carried out in dimensionless variables u_i and u_j such that

$$u_i = \frac{x}{h_i}, \text{and } u_j = \frac{y}{h_j}. \tag{3}$$

Note that $2h_i$ and $2h_j$ are the dimensions of node (i,j) in the x and y directions respectively. Since the coordinate system is located at the center of each node, u_i and u_j vary between -1 and +1, in a given node. This is advantageous since it would allow the use of the orthogonal properties of the Legendre polynomials.

The multigroup neutron diffusion equation is now rewritten in the dimensionless variables as,

$$D^g(i,j)\left[\frac{\partial^2 f^g(u_i,u_j)}{h_i^2 \partial u_i^2} + \frac{\partial^2 f^g(u_i,u_j)}{h_j^2 \partial u_j^2}\right] - \Sigma_t^g(i,j) f^g(u_i,u_j) +$$

$$\sum_{h=1}^{G} a^{gh}(i,j) f^h(u_i,u_j) = 0, \tag{4}$$

It is further assumed that the neutronic properties are constant over node (i,j). The multigroup neutron flux is now expanded using the dimensionless variables u_i and u_j. In particular, the expansion takes the following form in the nodal coordinate system,

$$f^g(u_i,u_j) = \sum_{m=0}^{M} \sum_{n=0}^{M-m} a_{m,n}^g(i,j) P_n(u_j) P_m(u_i), \tag{5}$$

where the P's are the Legendre polynomial expansion functions.

There are (M+1)(M+2)/2 unknown polynomial coefficients, $a^{g}_{m,n}(i,j)$, in equation (5) that must be determined for each node (i,j) and neutron group g. Therefore, a total of (M+1)(M+2)/2 linear independent equations are needed for each node and neutron group. In order to find this set of equations, the approximate solution in (5) is used in the multigroup neutron diffusion equation (4). The second derivatives of the approximate solution in (5) with respect to u_i and u_j are,

$$\frac{\partial^2 f^{g}(u_i,u_j)}{\partial u_i^2} = \sum_{m=0}^{M-2} \sum_{n=0}^{M-m-2} b^{g}_{m,n}(i,j)\, P_n(u_j)\, P_m(u_i), \tag{6}$$

$$\frac{\partial^2 f^{g}(u_i,u_j)}{\partial u_j^2} = \sum_{m=0}^{M-2} \sum_{n=0}^{M-m-2} c^{g}_{m,n}(i,j)\, P_n(u_j)\, P_m(u_i), \tag{7}$$

where

$$b^{g}_{m,n}(i,j) = \sum_{k=m+1}^{M-n} \frac{(2m+1)(k-m)(k+m+1)}{2}\, a^{g}_{k,n}(i,j), \tag{8}$$

if m = even, k = even,

if m = odd, k = odd,

and

$$c^{g}_{m,n}(i,j) = \sum_{k=n+1}^{M-m} \frac{(2n+1)(k-n)(k+n+1)}{2}\, a^{g}_{m,k}(i,j), \tag{9}$$

if n = even, k = even,

if n = odd, k = odd.

The relations in (6), and (7) along with (5) are inserted into the multigroup

diffusion equation (4). Since the approximate solution (5) and it's derivatives (6) and (7) do not exactly satisfy equation (4), a residual is defined as,

$$D^{g}(i,j)\sum_{m=0}^{M-2}\sum_{n=0}^{M-m-2}\left[\frac{b^{g}_{m,n}(i,j)}{h_i^2}+\frac{c^{g}_{m,n}(i,j)}{h_j^2}\right]P_n(u_j)P_m(u_i)$$

$$-\sum_{t}^{g}(i,j)\sum_{m=0}^{M}\sum_{n=0}^{M-m}a^{g}_{m,n}(i,j)P_n(u_j)P_m(u_i)$$

$$+\sum_{m=0}^{M}\sum_{n=0}^{M-m}\sum_{h=1}^{G}a^{gh}(i,j)\,a^{h}_{m,n}(i,j)P_n(u_j)P_m(u_i)=R^{g}(i,j). \qquad (10)$$

Equation (10) is further rearranged as:

$$D^{g}(i,j)\sum_{m=0}^{M-2}\sum_{n=0}^{M-m-2}d^{g}_{m,n}(i,j)P_n(u_j)P_m(u_i)$$

$$-\sum_{t}^{g}(i,j)\sum_{m=0}^{M}\sum_{n=0}^{M-m}a^{g}_{m,n}(i,j)P_n(u_j)P_m(u_i)$$

$$+\sum_{m=0}^{M}\sum_{n=0}^{M-m}b^{g}_{m,n}(i,j)P_n(u_j)P_m(u_i)=R^{g}(i,j) \qquad (11)$$

where,

$$d^{g}_{m,n}(i,j)=\frac{b^{g}_{m,n}(i,j)}{h_i^2}+\frac{c^{g}_{m,n}(i,j)}{h_j^2}, \qquad (12)$$

$$b^{g}_{m,n}(i,j) = \sum_{h=1}^{G} a^{gh}(i,j)\, a^{h}_{m,n}(i,j). \tag{13}$$

Since the neutron flux in (5) is an approximate solution, the residual in (11) needs to be minimized. In particular, one needs to minimize the least-squares of the residuals over the nodal interval with respect to the polynomial coefficients $a^{g}_{m,n}(i,j)$ as,

$$\frac{\partial}{\partial a^{g}_{m,n}(i,j)} \int_{-1}^{+1} \partial u_i \int_{-1}^{+1} [R^{g}(i,j)]^2 \partial u_j = 0. \tag{14}$$

Note the limits of integrations are between -1 and +1 which facilitates the integration process since Legendre polynomials are orthogonal in the same range. This is in fact the reason for using the dimensionless variables u_i and u_j as defined in (3). If the least-squares minimization process in (14) is carried out with respect to every coefficient that appears in the expansion function, then a set of linear equations would result. However, some of the equations will not be independent form each other and in addition, a number of the coefficients may be zero. Therefore, the application of the least-squares minimization in this paper deviates from the conventional approach in the choice of the coefficients that will be minimized. In particular, the least-squares minimization is carried out with respect to the $a^{g}_{m,n}$ coefficients that appear in the Laplacian term of the expansion function; i.e. the coefficients that are contained in $d^{g}_{m,n}$ as shown in (12). Therefore, the least-squares minimization becomes:

$$\frac{\partial}{\partial a^{g}_{m,n}(i,j)} \int_{-1}^{+1} \partial u_i \int_{-1}^{+1} [R^{g}(i,j)]^2 \partial u_j = 0 \text{ , } m+n \le M-2, \tag{15}$$

which is further rearranged as,

$$\int_{-1}^{+1}\int_{-1}^{+1} R^{g}(i,j) \frac{\partial R^{g}(i,j)}{\partial d^{g}_{m,n}(i,j)} \partial u_i \partial u_j = 0, \; m+n \le M-2. \tag{16}$$

The relations that result from (16) are,

$$D^{g}(i,j)\,d^{g}_{m,n} - \sum_{t}^{g}(i,j)\,a^{g}_{m,n}(i,j) + b^{g}_{m,n}(i,j) = 0, \quad m+n \le M-2. \tag{17}$$

Substituting (12) and (13) into (17) results in the following:

$$D^{g}(i,j)\left[\frac{b^{g}_{m,n}(i,j)}{h_i^2} + \frac{c^{g}_{m,n}(i,j)}{h_j^2}\right] - \sum_{t}^{g}(i,j)\,a^{g}_{m,n}(i,j)$$

$$+ \sum_{h=1}^{G} a^{gh}(i,j)\,a^{h}_{m,n}(i,j) = 0, \quad m+n \le M-2, \tag{18}$$

where a^{gh} is given in equation (2). Rearranging equation (18) and using equation (2), the following equation is obtained:

$$D^{g}(i,j)\left[\frac{b^{g}_{m,n}(i,j)}{h_i^2} + \frac{c^{g}_{m,n}(i,j)}{h_j^2}\right] - \sum_{t}^{g}(i,j)\,a^{g}_{m,n}(i,j) =$$

$$- \sum_{h=1}^{G}\left[\frac{1}{l}\,c^{g}n\,\sum_{f}^{h}(i,j) + \sum_{s}^{gh}(i,j)\right] a^{h}_{m,n}(i,j), \quad m+n \le M-2, \tag{19}$$

Note that the right hand side of equation (19) is assumed to be known from a previous iteration. The coefficients $b^{g}_{m,n}(i,j)$, and $c^{g}_{m,n}(i,j)$ are given in equations (8) and (9) in terms of the unknown polynomial expansion coefficients

$a^{g}_{m,n}(i,j)$. Equation (19) results in M(M+1)/2 linear independent equations. An additional (M+1) equations are needed to solve for the (M+1)(M+2)/2 polynomial coefficients of each node (i,j) and neutron group g. The additional equations are obtained from the interface conditions as described below .

3. NODAL INTERFACE CONDITIONS

The nodal interface conditions that are used in the current development is based on the extension of the 1-D partial currents to the 2-D case. However, before the development of interface conditions are presented, it should be noted that since in the 2-D case there are 4 surfaces, then an even number of interface equations will always be obtained.

The interface conditions will cause a problem since it will not produce the necessary number of equations to completely solve for the polynomial coefficients. The general form of the 2-D interface conditions are obtained from the 1-D partial currents given by Duderstadt and Hamilton (1976). Since the partial currents can not be satisfied at every point on the interfaces between two nodes, then the average value will be required to be continuous at the nodal interface. The 2-D partial currents at the interfaces are,

$$\int_{u_j(h)}^{u_j(h+1)} [-a f^{g}(u_i,u_j) - b\frac{1}{h_i}\frac{\partial f^{g}(u_i,u_j)}{\partial u_i}]_{u_i=+1} du_j = J^{g}_{-lh}(i+1,j), \qquad (20)$$

$$\int_{u_j(h)}^{u_j(h+1)} [+a f^{g}(u_i,u_j) - b\frac{1}{h_i}\frac{\partial f^{g}(u_i,u_j)}{\partial u_i}]_{u_i=-1} du_j = J^{g}_{+rh}(i-1,j), \qquad (21)$$

$$\int_{u_i(h)}^{u_i(h+1)} [-a f^{g}(u_i,u_j) - b\frac{1}{h_j}\frac{\partial f^{g}(u_i,u_j)}{\partial u_j}]_{u_j=+1} du_i = J^{g}_{-bh}(i,j+1), \qquad (22)$$

$$\int_{u_i(h)}^{u_i(h+1)} [+a f^{g}(u_i,u_j) - b\frac{1}{h_j}\frac{\partial f^{g}(u_i,u_j)}{\partial u_j}]_{u_j=-1} du_i = J^{g}_{+th}(i,j-1), \qquad (23)$$

where a =1/4, b =1/2 and h is the number of divisions on the nodal interface. The partial currents on the left of equations (20) through (23) are defined as:

$J_{-lh}(i+1, j)$ = The incoming partial current or currents from node (i+1,j) into node (i,j). This is the interface on the right of node (i,j),

$J_{+rh}(i-1, j)$ = The incoming partial current or currents from node (i-1,j) into node (i,j). This is the interface on the left of node (i,j),

$J_{-bh}(i, j+1)$ = The incoming partial current or currents from node (i,j+1) into node (i,j). This is the interface on the top of node (i,j),

$J_{+th}(i, j-1)$ = The incoming partial current or currents from node (i,j-1) into node (i,j). This is the interface on the bottom of node (i,j).

The integration in equations (20) through (23) contain a variable h, and as stated previously, it represents the number of divisions on a given nodal interface. The number of divisions depends on the order of the polynomial expansion, M, used to approximate the neutron flux in equation (5) and is:

If M = even, then: h = $1,2,...,\frac{M}{2}$,

$$u_i(h+1) - u_i(h) = u_j(h+1) - u_j(h) = \frac{4}{M},\ u_i(1) = u_j(1) = -1,$$

$$u_i\left(\frac{M}{2}\right) = u_j\left(\frac{M}{2}\right) = +1.$$

If M = odd, then: h = 1,2,...,$\frac{(M+1)}{2}$,

$$u_i(h+1) - u_i(h) = u_j(h+1) - u_j(h) = \frac{4}{(M+1)},\ u_i(1) = u_j(1) = -1,$$

$$u_i\left(\frac{M+1}{2}\right) = u_j\left(\frac{M+1}{2}\right) = +1.$$

From the above description of the number of divisions on each nodal interface, it is concluded that the same number of partial current relations are obtained for two subsequent expansion orders.

4. CONCLUSION

The fourth-order Legendre Polynomial expansion was used in this study with 9 nodes in each of the x and y directions. The number of unknown polynomial expansions that must be determined are 15 which requires the same number of independent equations. Of these, ten equations are obtained from the least-squares minimization while four equations are obtained from the interface conditions. This results in a total of 14 independent equations which is one equation less than the required 15. As a result, the polynomial coefficient $a^g_{2,2}(i,j)$, which appears the least in these equations, is set equal to zero for all nodes and neutron groups.

The results of the thermal flux profile, along the x-axis, is shown in Fig. 2 for the IAEA 2-D benchmark problem(Argonne Code Center, 1977) while Fig. 3 shows the distribution of the thermal flux. The results of the finite-difference solution using the CITATION (1979) and the GNOMER (1994) codes are also shown in Fig.2. It is noted that the CITATION results in a finite-difference solution while the GNOMER, using Green's function, results in a nodal solution. The eigenvalue of the presented nodal model is 1.02996, while for the finite-difference and Green's function nodal models are 1.02964 and 1.02975 respectively.

It is observed from the results that the presented nodal model matches the results of both the finite-difference and the other nodal model at all the regions except the core-reflector interface. It is also observed that extending the 1-D partial currents to the 2-D case, at the interfaces, is natural and easy to use.

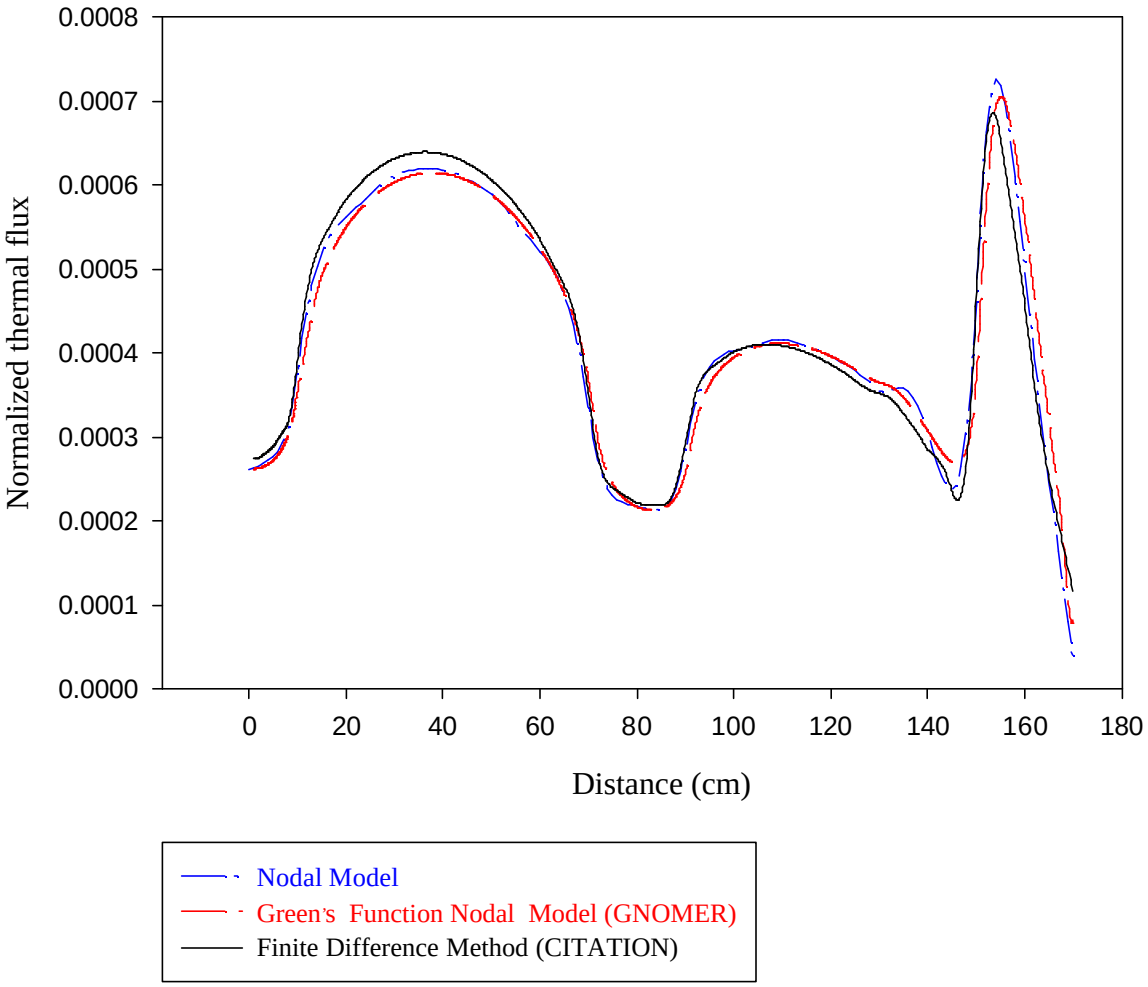

Fig. 2. Thermal flux distribution of the IAEA-2D benchmark

Therefore, it can be concluded that accurate results can be expected in all cases except where severe flux gradients occur. In these cases, one can either increase the number of nodes or use a higher order polynomial expansion.

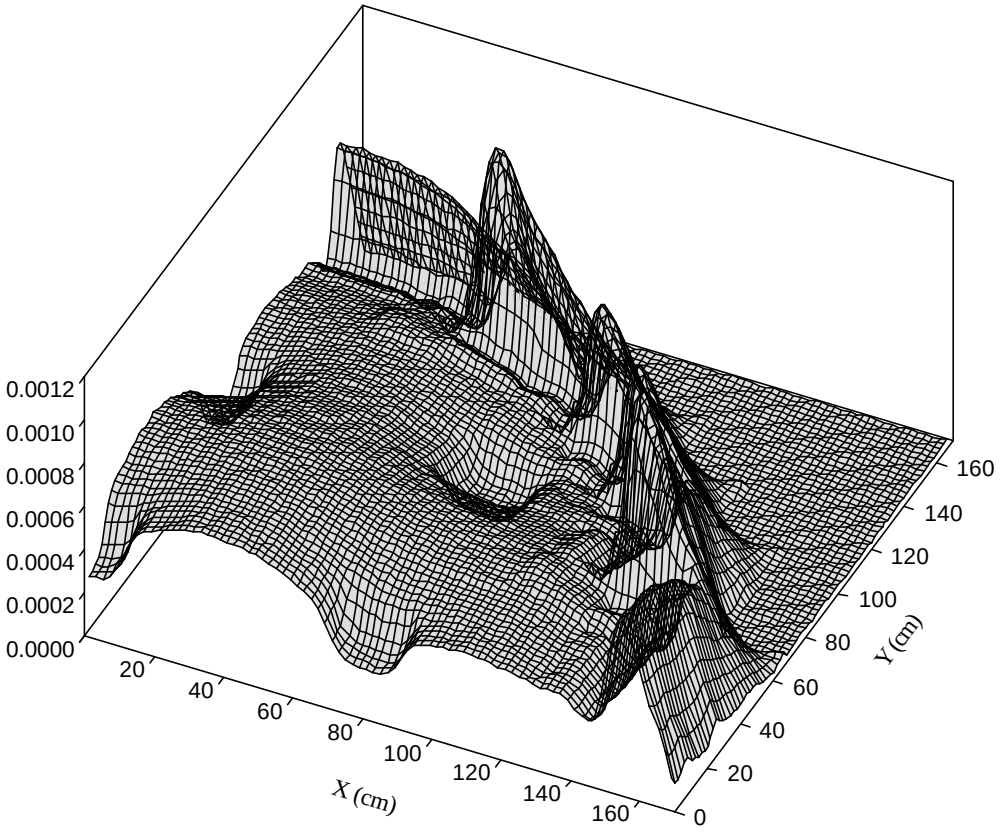

Fig.3 . Normalized thermal flux distribution of the IAEA-2D benchmark problem

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