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Use of pseudo-harmonics method coupled with finite differences coarse mesh in the solution of fixed source problems

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Abstract

A method based in the pseudo-harmonics method was developed to solve the fixed source problem. The pseudo-harmonics method is based on the eigenfunctions associated with the leakage and removal matrix operator of the neutron diffusion equation, which will be treated here in three dimensions and two groups of energy. This matrix is built in this work through the nodal discretization supplied by coarse mesh finite differences method (CMFDM). CMFDM has as input data the average currents and the average fluxes in the faces of the node, and the average flux in the node, previously obtained by the nodal expansion method. The results obtained with the pseudo-harmonics procedure show good accuracy when compared to the reference results of the source problem tested. Moreover, it is a method which can be easily implemented to solve this type of problems.

1. Introduction

The fixed source problem, or source problem for short, is usually represented by a non-homogeneous linear system of equations. The solution of this system can be

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obtained by direct inversion of the coefficient matrix. This direct solution method is, however, inefficient, since the system matrix is sparse and one usually solves the problem by iterative methods or, alternatively, making use of the associated (homogeneous) eigenvalue problem. Nodal methods for solving the steady-state neutron diffusion eigenvalue equation are well established in nuclear reactor physics, nowadays and they can also be used to obtain solutions of the source problem, since it is reasonable to suppose that the solution can be expressed as an expansion in eigenfunctions of the matrix operator of the linear system. In this context, we may use as a basis the pseudo-harmonics of the system, which are defined as the eigenfunctions of the leakage plus removal operators of the problem.

In the development of perturbation theory applied to reactor physics problems, the pseudo-harmonics method has emerged as a viable alternative to overcome some difficulties appearing in the determination of the neutron flux in perturbative computations (Gomit et al., 1985; da Silva et al., 1988; de Abreu et al., 1989). Even though this method originated from perturbative studies, it has also been successful for solving non perturbative problems, such as in the solution of fixed source problems with importance functions or auxiliary functions (de Lima et al., 2004). One should also note that this method has also been successfully applied in conjunction with coarse mesh nodal methods (Claro and Alvim, 1991).

In the work of de Lima et al. (2004) the pseudo-harmonics method is successfully applied together with the flux expansion method (FEM) to the solution of problems involving auxiliary functions. However, due to FEM construction, the matrix that determines the pseudo-harmonics includes the average surface fluxes in addition to the nodal fluxes, thus introducing a greater number of variables to be determined. In practice this amounts to calculating three eigenvectors for each node, in 2D calculations, and four in the 3D case.

Among coarse mesh methods, the coarse mesh finite differences method (CMFDM) is of interest to our work since, due to its structure, it is easy to construct the leakage + removal matrix and, differently from FEM, it is not necessary to calculate face averaged nodal fluxes. The CMFDM makes use of the results from the nodal expansion method (NEM). In practice, we will use the NEM results and the pseudo-harmonics generated via CMFDM only once, to solve a linear system for any of the source problems described in this work.

In the next section, we present the CMFDM and how the continuity equation is discretized by this method. In Section 3, we present solutions obtained with the pseudo-harmonics method. Section 4 shows the results obtained and finally in Section we present the conclusions of this work.

2. Coarse mesh finite differences method

The coarse mesh finite differences here developed is based on the formulation proposed by Aragones and Ahnert (1986) and in the work of Pereira et al. (2002), which explored the fact that CMFDM maintains the general structure of the classical finite difference method in order to obtain the mathematical adjoint fluxes.

The method uses as input data the diffusion coefficient $D_g^{i,j,k}$, the nodal face averaged currents $J_{gus}^{i,j,k}$, the face averaged nodal fluxes $\psi_{gus}^{i,j,k}$ ($s = e, d$) and the nodal averaged fluxes $\phi_g^{i,j,k}$, previously computed by the nodal expansion method (Martinez et al., 1999).

According to this formulation, adopting the coarse mesh correction factors that modify the finite differences fine mesh formulation, we can write the nodal face averaged currents in the following way:

$$J_{gue}^{i,j,k} = -\frac{2}{a_u^r} D_g^{i,j,k} \left(\phi_g^{i,j,k} - \psi_{gue}^{i,j,k} \right) + C_{gue}^{i,j,k} \left(\phi_g^{i,j,k} + \psi_{gue}^{i,j,k} \right) \tag{1}$$

and

$$J_{gud}^{i,j,k} = -\frac{2}{a_u^r} D_g^{i,j,k} \left(\psi_{gud}^{i,j,k} - \phi_g^{i,j,k} \right) - C_{gud}^{i,j,k} \left(\phi_g^{i,j,k} + \psi_{gud}^{i,j,k} \right), \tag{2}$$

where $C_{gus}^{i,j,k}$ are correction factors and a_u^r is the node dimension in direction u, with $g = 1$ and 2 representing energy groups, $u = x$, y, z the Cartesian coordinates, $s = e$, d left and right node faces, i, j, k a generic node and

$$r \equiv \begin{cases} i & \text{for } u = x, \\ j & \text{for } u = y, \\ k & \text{for } u = z. \end{cases}$$

According to Eqs. (1) and (2) and knowing $J_{gus}^{i,j,k}$, $\psi_{gus}^{i,j,k}$, $\phi_g^{i,j,k}$, $D_g^{i,j,k}$ and a_u^r we can determine the correction factors by

$$C_{gue}^{i,j,k} = \frac{J_{gue}^{i,j,k} + \frac{2}{a_u^r} D_g^{i,j,k} \left(\phi_g^{i,j,k} - \psi_{gud}^{i,j,k} \right)}{\phi_g^{i,j,k} + \psi_{gue}^{i,j,k}} \tag{3}$$

and

$$C_{gud}^{i,j,k} = \frac{J_{gud}^{i,j,k} - \frac{2}{a_u^r} D_g^{i,j,k} \left(\phi_g^{i,j,k} - \psi_{gud}^{i,j,k} \right)}{\phi_g^{i,j,k} + \psi_{gud}^{i,j,k}}. \tag{4}$$

Using continuity of fluxes and currents at node interfaces, we can write, e.g., for three consecutive nodes in x-direction

$$J_{gxe}^{i,j,k} = -D_{gxe}^{i,j,k} \phi_g^{i,j,k} + D_{gxd}^{i-1,j,k} \phi_g^{i-1,j,k} \tag{5}$$

and

$$J_{gxd}^{i,j,k} = D_{gxd}^{i,j,k} \phi_g^{i,j,k} - D_{gxe}^{i+1,j,k} \phi_g^{i+1,j,k}, \tag{6}$$

where

$$D_{gxe}^{i,j,k} = \frac{2 \left(\frac{1}{a_x^{i-1}} D_g^{i-1,j,k} + \frac{1}{2} C_{gxd}^{i-1,j,k} \right) \left(\frac{1}{a_x^i} D_g^{i,j,k} - \frac{1}{2} C_{gxe}^{i,j,k} \right)}{\left(\frac{1}{a_x^{i-1}} D_g^{i-1,j,k} + \frac{1}{2} C_{gxd}^{i-1,j,k} \right) + \left(\frac{1}{a_x^i} D_g^{i,j,k} + \frac{1}{2} C_{gxe}^{i,j,k} \right)} \tag{7}$$

and

$$D_{gxe}^{i,j,k} = \frac{2\left(\frac{1}{a_x^i} D_g^{i,j,k} - \frac{1}{2} C_{gxd}^{i,j,k}\right)\left(\frac{1}{a_x^{i+1}} D_g^{i+1,j,k} + \frac{1}{2} C_{gxe}^{i+1,j,k}\right)}{\left(\frac{1}{a_x^i} D_g^{i,j,k} + \frac{1}{2} C_{gxd}^{i,j,k}\right) + \left(\frac{1}{a_x^{i+1}} D_g^{i+1,j,k} + \frac{1}{2} C_{gxe}^{i+1,j,k}\right)}. \tag{8}$$

Analogously, we can determine the average currents and the diffusion coefficients at node faces, for directions y and z.

Considering the 3D neutron continuity equation, discretized with the NEM procedure, with two energy groups

$$\sum\nolimits_{u=x,y,z} \frac{1}{a_u^r}\left(J_{gud}^{i,j,k} - J_{gue}^{i,j,k}\right) + \sum_{Rg}^{i,j,k} \phi_g^{i,j,k} = \frac{1}{K_{\text{eff}}} \chi_g \sum_{g'=1}^{2} \nu \sum_{fg'}^{i,j,k} \phi_{g'}^{i,j,k} + \sum_{\substack{g'=1 \\ g'=g}}^{2} \sum_{gg'}^{i,j,k} \phi_{g'}^{i,j,k}, \tag{9}$$

where $\sum_{Rg}^{i,j,k}$, $\nu\sum_{fg'}^{i,j,k}$ and $\sum_{gg'}^{i,j,k}$ are, respectively, node averaged microscopic cross sections for removal, fission and scattering.

Using Eqs. (5) and (6) and their analogous in y and z in Eq. (9), we have

$$\begin{aligned}
&-\frac{1}{a_z^k} D_{gzd}^{i,j,k-1} \phi_g^{i,j,k-1} - \frac{1}{a_y^j} D_{gyd}^{i,j-1,k} \phi_g^{i,j-1,k} - \frac{1}{a_x^i} D_{gxd}^{i-1,j,k} \phi_g^{i-1,j,k} \\
&\quad + \sum\nolimits_{u=x,y,z} \frac{1}{a_u^r}\left(D_{gue}^{i,j,k} + D_{gud}^{i,j,k}\right) \phi_g^{i,j,k} - \frac{1}{a_x^i} D_{gxe}^{i+1,j,k} \phi_g^{i+1,j,k} \\
&\quad - \frac{1}{a_y^j} D_{gye}^{i,j+1,k} \phi_g^{i,j+1,k} - \frac{1}{a_z^k} D_{gze}^{i,j,k+1} \phi_g^{i,j,k+1} \\
&\qquad = \frac{1}{K_{\text{eff}}} \chi_g \sum_{g'=1}^{2} \nu \sum_{fg'}^{i,j,k} \phi_{g'}^{i,j,k} + \sum_{\substack{g'=1 \\ g'=g}}^{2} \sum_{gg'}^{i,j,k} \phi_{g'}^{i,j,k}.
\end{aligned} \tag{10}$$

Putting Eq. (10), as explained in Fig. 1, in matrix form one has

$$\begin{aligned}
&-B_{n,q}\phi_g^{i,j,k-1} - B_{n,t}\phi_g^{i,j-1,k} - B_{n,p}\phi_g^{i-1,j,k} - B_{n,n}\phi_g^{i,j,k} \\
&-B_{n,\alpha}\phi_g^{i+1,j,k} - B_{n,\beta}\phi_g^{i,j+1,k} - B_{n,\gamma}\phi_g^{i,j,k+1} = \frac{1}{K_{\text{eff}}} F^{i,j,k}\phi_{g'}^{i,j,k} + S^{i,j,k}\phi_{g'}^{i,j,k},
\end{aligned} \tag{11}$$

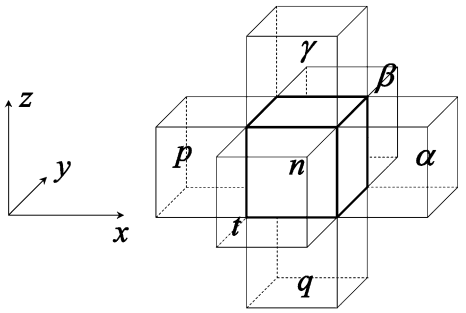

Fig. 1. Generic node and neighbors in directions x, y, z.

where

$$F^{i,j,k} \equiv \begin{bmatrix} \chi_1 v \sum\limits_{f1}^{i,j,k} & \chi_1 v \sum\limits_{f2}^{i,j,k} \\ \chi_2 v \sum\limits_{f1}^{i,j,k} & \chi_2 v \sum\limits_{f2}^{i,j,k} \end{bmatrix},$$

$$S^{i,j,k} \equiv \begin{bmatrix} 0 & \sum\limits_{12}^{i,j,k} \\ \sum\limits_{21}^{i,j,k} & 0 \end{bmatrix},$$

$$B_{n,m} \equiv \begin{bmatrix} b^1_{l,m} & 0 \\ 0 & b^2_{l,m} \end{bmatrix},$$

$$B_{n,n} \equiv \begin{bmatrix} b^1_{n,n} & 0 \\ 0 & b^2_{n,n} \end{bmatrix}$$

with

$$b^g_{n,n} \equiv \sum_{Rg}^{i,j,k} + \sum_{u=x,y,z} \frac{1}{a^r_u} \left(D^{i,j,k}_{gue} - D^{i,j,k}_{gud} \right),$$

and with n representing node i, j, k and m being its left (p) ou right (α) neighbor, in direction x, in front (t) or behind (β), in direction y, and below (q) or above (γ), in direction z. For the left neighbor one has

$$b^g_{n,m} \equiv \frac{1}{a^i_x} D^{i-1,j,k}_{gxd}.$$

By convenience, we can put Eq. (11) in block-heptadiagonal matrix form

$$[B] \underset{\sim}{\Phi} = [S] \underset{\sim}{\Phi} + \frac{1}{K_{\text{eff}}} [F] \underset{\sim}{\Phi} \tag{12}$$

with

$$\underset{\sim}{\Phi} \equiv \begin{pmatrix} \underset{\sim_1}{\phi} \\ \underset{\sim_2}{\phi} \end{pmatrix}, \quad \underset{\sim_g}{\phi} \equiv \begin{pmatrix} \phi^{i,j,k-1}_g \\ \phi^{i,j-1,k}_g \\ \phi^{i-1,j,k}_g \\ \phi^{i,j,k}_g \\ \phi^{i+1,j,k}_g \\ \phi^{i,j+1,k}_g \\ \phi^{i,j,k+1}_g \end{pmatrix}, \quad (g = 1, 2),$$

$$[B] \equiv \begin{bmatrix} B_1 & 0 \\ 0 & B_2 \end{bmatrix},$$

where

$$B_g \equiv \begin{pmatrix} b^g_{1,1} & b^g_{1,2} & & & b^g_{1,n} & & & b^g_{1,N-1} & \\ b^g_{2,1} & b^g_{2,2} & b^g_{2,3} & & & b^g_{2,n+1} & & & b^g_{2,N} \\ & b^g_{3,2} & b^g_{3,3} & \ddots & & & \ddots & & \\ & & \ddots & \ddots & b^g_{n-1,n} & & & b^g_{n-1,N-1} & \\ b^g_{n,1} & & & \ddots & b^g_{n,n} & \ddots & & & b^g_{n,N} \\ & b^g_{n+1,2} & & & b^g_{n+1,n} & \ddots & \ddots & & \\ & & \ddots & & & \ddots & b^g_{N-2,N-2} & b^g_{N-2,N-1} & \\ b^g_{N-1,1} & & & b^g_{N-1,n-1} & & & b^g_{N-1,N-2} & b^g_{N-1,N-1} & b^g_{N-1,N} \\ & b^g_{N,1} & & & b^g_{N,n} & & & b^g_{N,N-1} & b^g_{N,N} \end{pmatrix}, \quad (g=1,2)$$

with N being the total number of nodes. The scattering and fission matrices are, respectively

$$[S] \equiv \begin{bmatrix} 0 & S_1 \\ S_2 & 0 \end{bmatrix} \quad \text{and} \quad [F] \equiv \begin{bmatrix} F_{11} & F_{12} \\ F_{21} & F_{22} \end{bmatrix}$$

with block-diagonal elements of dimension $N \times N$.

3. Pseudo-harmonic expansions

To solve a linear system of the form

$$[B]^{\mathrm{S}} \underset{\sim}{\Phi} = \underset{\sim}{Q}, \tag{13}$$

where $[B]^{\mathrm{S}}$ is the symmetrical part of matrix $[B]$ and $\underset{\sim}{Q}$ represents any source matrix, we can, alternatively, use eigenfunctions expansions. In this work, we will use as eigenfunctions the pseudo-harmonics, which are the eigenfunctions generated by the operator representing leakage + removal for the g energy group (matrix $[B^s_g]$, $g = 1, 2$).

A characteristic of the pseudo-harmonics method is that the eigenfunctions are obtained for each group, via uncoupled equations. Assuming that the solution to Eq. (13) is given by the expansion

$$\underset{\sim}{\Phi} = \begin{bmatrix} \underset{\sim}{\phi}_1 \\ \underset{\sim}{\phi}_2 \end{bmatrix} = \sum_{i=1}^{N} \left(c_{i,1} \begin{bmatrix} \underset{\sim}{\omega}_{1,i} \\ 0 \end{bmatrix} + c_{i,2} \begin{bmatrix} 0 \\ \underset{\sim}{\omega}_{2,i} \end{bmatrix} \right), \tag{14}$$

where $\underset{\sim g,j}{\omega}$ are eigenfunctions of the following eigenvalue problem:

$$\left[B_g^{\mathrm{S}}\right] \underset{\sim g,j}{\omega} = \lambda_{g,j} \underset{\sim g,j}{\omega} \tag{15}$$

and substituting Eq. (14) into Eq. (13) and using Eq. (15), one has

$$[B^{\mathrm{S}}] \underset{\sim}{\Phi} = \sum_{i=1}^{N} \left(c_{i,1} \begin{bmatrix} \lambda_{1,i} \underset{\sim 1,i}{\omega} \\ \underset{\sim}{0} \end{bmatrix} + c_{i,2} \begin{bmatrix} \underset{\sim}{0} \\ \lambda_{2,i} \underset{\sim 2,i}{\omega} \end{bmatrix} \right) = \begin{bmatrix} \underset{\sim 1}{Q} \\ \underset{\sim 2}{Q} \end{bmatrix}. \tag{16}$$

Since the pseudo-harmonics form an orthogonal set, due to the symmetry of matrix $[B_g^{\mathrm{S}}]$, that is

$$\left\langle \overset{T}{\underset{\sim g,j}{\omega}} \; \underset{\sim g,i}{\omega} \right\rangle = 0 \quad \text{for} \quad j \neq i,$$

we can multiply Eq. (16) by $\overset{T}{\underset{\sim g,j}{\omega}}$ and integrate the resulting equation to obtain the expansion coefficients (14) and consequently the solution of system (13)

$$c_{i,l} = \frac{\left\langle \overset{T}{\underset{\sim g,i}{\omega}} \; \underset{\sim g}{Q} \right\rangle}{\lambda_{l,i} \left\langle \overset{T}{\underset{\sim g,i}{\omega}} \; \underset{\sim g,i}{\omega} \right\rangle}, \quad g = 1, 2.$$

To obtain eigenvalues and eigenfunctions for this method we have made use of the well-known Jacobi method.

We have verified that matrix $[B]$, representing leakage + removal, in the LHS of Eq. (10), is slightly unsymmetrical. Since the method of pseudo-harmonics requires that the eingenfunctions be calculated from a symmetric matrix, one has to obtain its symmetric part, by writing $[B]$ as the sum of a symmetric and an anti-symmetric matrix, as shown below

$$[B] = [B]^{\mathrm{S}} + [B]^{\mathrm{A}}, \tag{17}$$

3	2	2	2	3	2	2	1	4
2	2	2	2	2	2	2	1	4
2	2	2	2	2	2	1	1	4
2	2	2	2	2	2	1	4	4
3	2	2	2	3	1	1	4	
2	2	2	2	1	1	4	4	
2	2	1	1	1	4	4		
1	1	1	4	4	4			
4	4	4	4					

Fig. 2. Quarter-core symmetry for IAEA-3D reactor.

where

$$[B]^{S} \equiv \frac{[B] + [B]^{T}}{2}$$

and

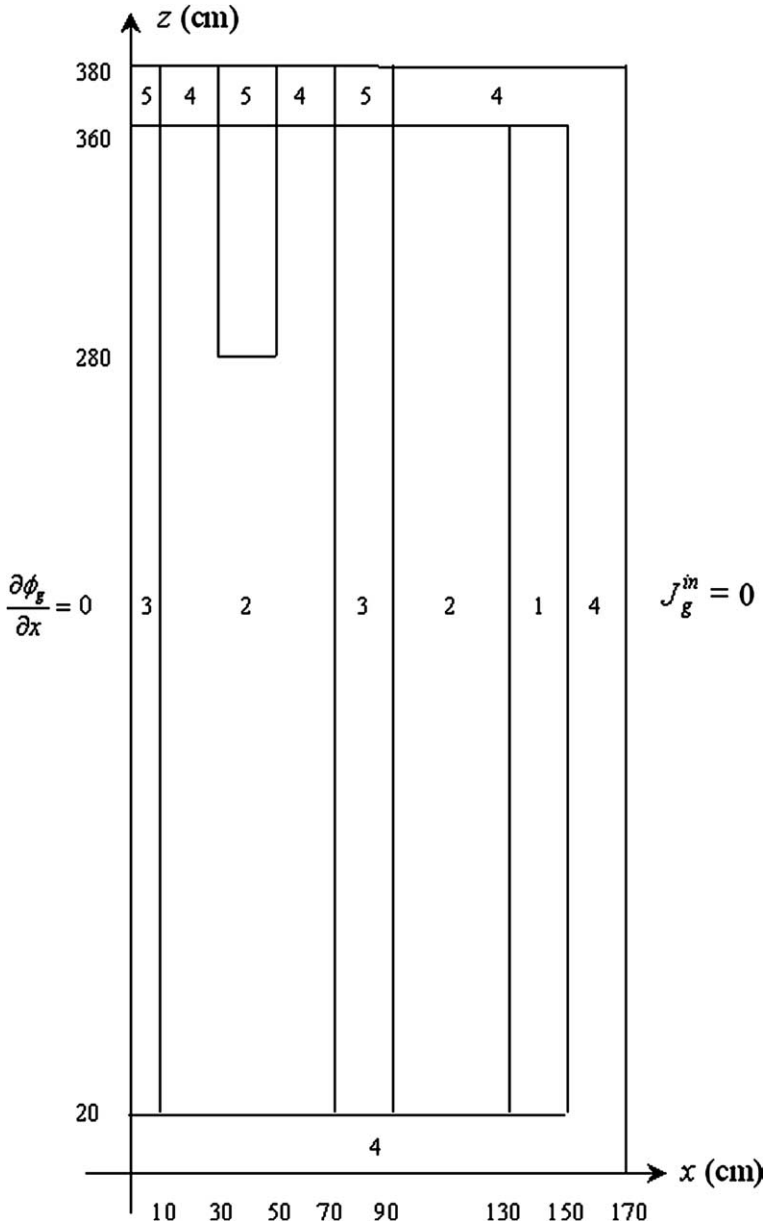

Fig. 3. IAEA-3D reactor core.

$$[B]^{\mathrm{A}} \equiv \frac{[B]-[B]^{T}}{2}.$$

Substituting Eq. (17) into Eq. (12), one has

$$[B]^{\mathrm{S}} \underset{\sim}{\Phi} = [S] \underset{\sim}{\Phi} + \frac{1}{K_{\mathrm{eff}}} [F] \underset{\sim}{\Phi} - [B]^{\mathrm{A}} \underset{\sim}{\Phi}$$

or

$$[B]^{\mathrm{S}} \underset{\sim}{\Phi} = \underset{\sim}{Q}, \tag{18}$$

Table 1
Multigroup nuclear constants

Type	g	D_g	$\sum_{ag}$	$\nu\sum_{fg}$	$\sum_{gg'}$
1	1	1.5	0.01	0.0	0.02
	2	0.4	0.08	0.135	0.0
2	1	1.5	0.01	0.0	0.02
	2	0.4	0.085	0.135	0.0
3	1	1.5	0.01	0.0	0.02
	2	0.4	0.13	0.135	0.0
4	1	2.0	0.0	0.0	0.04
	2	0.3	0.01	0.0	0.0
5	1	2.0	0.0	0.0	0.04
	2	0.3	0.055	0.0	0.0

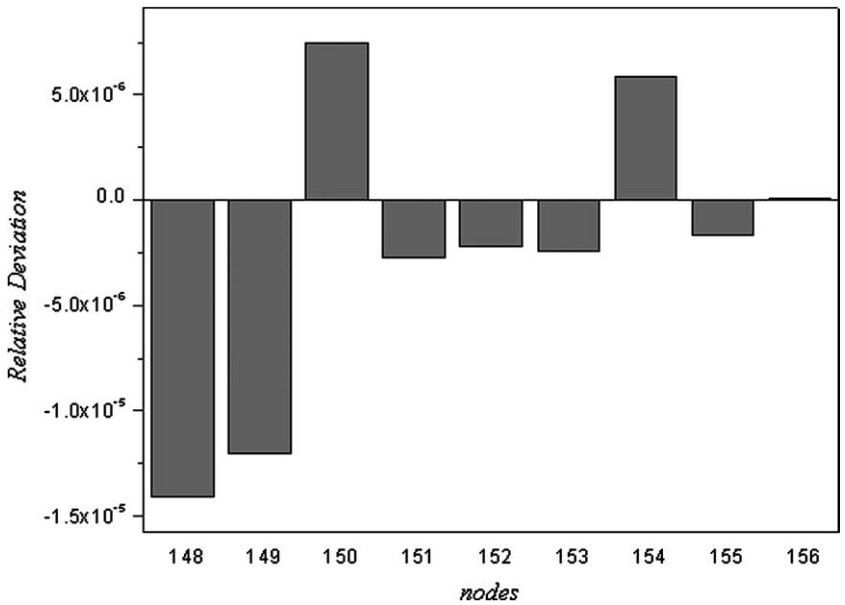

Fig. 4. Relative error at row containing node 148.

where

$$[B]^{S} \equiv \begin{bmatrix} B_1^S & 0 \\ 0 & B_2^S \end{bmatrix}$$

and

$$\underset{\sim}{Q} \equiv [S] \underset{\sim_{dir}}{\Phi} + \frac{1}{K_{eff}}[F] \underset{\sim_{dir}}{\Phi} - [B]^{A} \underset{\sim_{dir}}{\Phi}, \tag{19}$$

where the flux $\underset{\sim_{dir}}{\Phi}$ is the solution of Eq. (12), directly obtained by the CMFD method.

4. Results

The system described by Eq. (18), with the source term given by Eq. (19) was used to test the expansion in pseudo-harmonics to solve source problems. Let us consider as reference vectors the average nodal fluxes obtained with CMFDM. In our test we used the IAEA-3D problem, with 1/4 symmetry, with two groups of energy. Fig. 2 shows this symmetry in a *xy* plane of the reactor core. Fig. 3 shows a *xz* plane with the control bank positions (BBC) and also the boundary and continuity conditions used.

The nuclear constants for two energy groups are shown in Table 1, where we made the following description: Types 1 and 2 represent fuel without BBC, Type 3 fuel with BBC, Type 4 superior, inferior and side reflectors without BBC and Type 5 superior reflector with BBC. For the fission spectrum we have adopted $\chi_1 = 1.0$ and $\chi_2 = 0.0$.

Using this pseudo-harmonics method the results of the linear system given by Eq. (14) were practically the same as the reference values calculated by CMFD. The largest relative error was of approximately $10^{-5}\%$, in node number 148, in the thermal group. Fig. 4 shows the relative error in the line that contains the referred node.

5. Conclusions

The results obtained with the pseudo-harmonics procedure show good accuracy when compared to the reference results of the source problem tested. Besides that, it is a method that can be easily implemented to solve this type of problems. In practical terms, it is possible to construct a coarse mesh finite differences method, aiming only at getting the leakage + removal matrix, which is the one needed for the pseudo-harmonics method. In this work, although the CMFDM has been adapted to obtain only the leakage + removal matrix, it retained its original purpose of calculating k_{eff}, the average nodal fluxes and the mathematical adjoint fluxes and the average nodal fluxes obtained with it were considered the reference values for the source problem treated.

In view of the good performance shown here for the pseudo-harmonics method, one has to consider its application to source problems in Reactor Physics and not necessarily only to perturbative problems.

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