SOLUTION OF THE SPATIAL KINETIC EQUATIONS USING THE EXPANSION IN PSEUDO-HARMONICS: CASES 1D and 2D

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ABSTRACT

Recently was demonstrated that the steady-state fixed source problems, usually represented by a non homogeneous linear system of equations, can be solved by the method of the pseudo-harmonics. The method of the pseudo-harmonics is based on the eigenfunctions associated with the leakage and removal matrix operator of the neutron diffusion equation. In this case the fixed source problem was solved considering that the neutron flux can be expanded in these eigenfunctions. The method of the pseudo-harmonics was just summarized in the determination of the coefficients of the expansion of the neutron flux, substituting like this an scheme of numeric inversion of the matrix of the linear system, usually employee in this problem type.

The present work has as objective of study the possibility of to apply the method of the pseudo-harmonic in the solution of the linear system, which appears starting from the discretization of the equations of the spatial kinetic. For so much the same basic idea used in the solution of the fixed source problem was adopted now for the spatial kinetic.

The method was tested for the cases 1D and 2D, formulated to leave of the discretization in finite differences of the kinetic spatial equations. The method showed good results when compared with the direct method.

Key Words: Fixed Source, Spatial Kinetic, Pseudo-Harmonics.

1. INTRODUCTION

The conventional methods of solution of the equations of the spatial kinetics, of the theory of diffusion of neutrons, usually request the implicit solution of a linear system so that the kinetic matrix should be inverted numerically in each step in the evolution of the time. Such a numeric inversion corresponds to the process that demands the largest computational cost in the methods for the spatial kinetics. To avoid the use of those processes the explicit methods they can be applied in the solution of the equations of the space kinetics, because the same ones don't involve
the numeric inversion. However to obtain a convergent and stable solution with the explicit methods, it is necessary to use steps in the time with a much smaller size than in the implicit methods, and with that, generating a prohibitive computational cost.

In this work the alternative application of an expansion method is demonstrated with base in special eigenfunctions in the solution of the equations of the spatial kinetics that it doesn't request the numeric inversion, without committing the effort computational. The proposed method is based on the work related in [1], where the stationary neutrons diffusion equation with the presence of fixed source was solved through an expansion in pseudo-harmonics. By definition the pseudo-harmonics are the eigenfunctions associated to the matrix of the operator that it contains the leakage plus removal of the stationary neutrons diffusion equation [2, 3]. For a spatial discretization implemented by finite differences the referred matrix is symmetrical. In this work the pseudo-harmonics will be calculated taking into account the symmetrical part of the kinetic matrix of the problem.

In the next section is described, in a brief way, a direct method of solution of the equations of the spatial kinetics based on the space discretization in finite differences and in an implicit scheme to treat the dependence in the time. This method will obtain the reference solutions for comparison ends. In the section 3 is shown as the expansion in pseudo-harmonics can be applied in the linear system that appears in the formalism of the direct method. In the section 4 the results are presented for two cases of a problem in one-dimension with two groups of energy and six groups of precursors and, finally, in the section 5 the conclusions.

2. SOLUTION OF THE SPATIAL KINETICS EQUATIONS

The equations of the spatial kinetics in the theory of neutrons diffusion for two groups of energy are written in the following form:

\[
\frac{1}{\nu_1} \frac{\partial}{\partial t} \phi_1(r,t) = \nabla D_1(r,t) \nabla \phi_1(r,t) - \sum_{R,1} \phi_1(r,t) \phi_1(r,t) + (1 - \beta) \sum_{g=1}^2 v \sum_{f,g} \phi_g(r,t) \phi_g(r,t) + \sum_{i=1}^6 \lambda_i c_i(r,t),
\]

(1)

\[
\frac{1}{\nu_2} \frac{\partial}{\partial t} \phi_2(r,t) = \nabla D_2(r,t) \nabla \phi_2(r,t) - \sum_{R,2} \phi_2(r,t) \phi_2(r,t) + \sum_{i=1}^6 \phi_1(r,t) \phi_1(r,t)
\]

and

\[
\frac{\partial}{\partial t} c_i(r,t) = \beta \sum_{g=1}^2 v \sum_{f,g} \phi_g(r,t) \phi_g(r,t) - \lambda_i c_i(r,t),
\]

(2)

where \(\phi_g(r,t)\) and \(c_i(r,t)\) are, respectively, the neutrons flux in the group \(g\) and the concentration of precursors of delayed neutrons in the group \(l\), both defined in the point \(r\) and in the time \(t\); with \(g = 1, 2\). To solve the equations (1) and (2) the same are discretized in the space and in the time.

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2.1. Spatial Discretization

The implementation of the spatial discretization can use the method of finite differences in the scheme centered in the mesh. This method leads to the following system of equations:

\[
[u]^{-1} \frac{d}{dt} \Phi(t) = -[B] \Phi(t) + (1 - \beta)[F] \Phi(t) + [S] \Phi(t) + \sum_{i=1}^{L} \lambda_i \xi_i(t),
\]

with

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

[F] = \begin{bmatrix}
F_{11} & F_{12} \\
0 & 0
\end{bmatrix},

[S] = \begin{bmatrix}
0 & 0 \\
S_{21} & 0
\end{bmatrix},
\]

with \([B_g](g = 1, 2)\) is tri-diagonal for the case 1D, representing the leakage plus removal, \([F]\) and \([S]\) are, respectively, the fission and scattering matrix, and they are formed by diagonal blocks, and

\[
\xi_i(t) = \begin{bmatrix}
C^i_1(t) \\
\vdots \\
C^i_{NP}(t)
\end{bmatrix},

\Phi(t) = \begin{bmatrix}
\phi_1(t) \\
\phi_2(t) \\
\vdots \\
\phi_{NP}(t)
\end{bmatrix},

\phi_i(t) = \text{col}[\phi^i_1(t), \ldots, \phi^i_{NP}(t)],
\]

with \(NP\) being the number of points used in the discretization.

2.2. Solution in the Time

To solve the ordinary differential equations dependent in the time, equations (3) and (4), two procedures of numeric integration are adopted. The first method integrates the equation of the concentration of precursors analytically, while the other treats the neutrons equation through the method of Implicit Euler [4]. Using the two procedures is arrived to the following system of linear equations:

\[
\begin{bmatrix}
T_{11} & T_{12} \\
T_{21} & T_{22}
\end{bmatrix}
\begin{bmatrix}
\phi_1^{(n+1)} \\
\phi_2^{(n+1)}
\end{bmatrix}
= \begin{bmatrix}
R_{11} & R_{12} \\
0 & R_{22}
\end{bmatrix}
\begin{bmatrix}
\phi_1^{(n)} \\
\phi_2^{(n)}
\end{bmatrix}
+ \sum_{i=1}^{L} \lambda_i e^{-\lambda_i \Delta t}
\begin{bmatrix}
\xi_i^{(n)} \\
0
\end{bmatrix},
\]

where the blocks of matrix are given for:

\[
[T_{11}] = [I] + \nu \Delta t \left([B_1]^{(n+1)} - \left(1 - \beta\right) + \sum_{i=1}^{L} \lambda_i \beta_i \right)[F_{11}]^{(n+1)}},
\]

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\[
[T_{12}] = -u_1 \Delta t \left( (1 - \beta) + \sum_{l=1}^{L} \lambda_l \beta_l b_l \right) [F_{12}]^{(n+1)},
\]
\[
[T_{21}] = -u_2 \Delta t [S_{21}]^{(n+1)},
\]
\[
[T_{22}] = [I] + u_2 \Delta t [B_2]^{(n+1)},
\]
\[
[R_{11}] = [I] + u_1 \Delta t \sum_{l=1}^{L} \lambda_l \beta_l a_l [F_{11}]^{(n)},
\]
\[
[R_{12}] = u_1 \Delta t \sum_{l=1}^{L} \lambda_l \beta_l a_l [F_{12}]^{(n)},
\]
\[
[R_{21}] = 0,
\]
\[
[R_{22}] = [I],
\]

and the factors \( a_l \) and \( b_l \) are given for

\[
a_l = \frac{1 + \lambda_l \Delta t (1 - e^{-\lambda_l \Delta t})}{\lambda_l^2 \Delta t} - \frac{1}{\lambda_l} \quad \text{e} \quad b_l = \frac{\lambda_l \Delta t - 1 + e^{-\lambda_l \Delta t}}{\lambda_l^2 \Delta t}.
\]

The index \( n \) that appears in the equations of (7) the (13) is the discretization index in the variable time. The system of linear equations in (7) it is solved iteratively, being accelerated for the process SOR [5].

3. APPLICATION OF THE EXPANSION IN PSEUDO-HARMONICS

To apply the expansion in pseudo-harmonics, the equation (7) is rewrite in the following form:

\[
\begin{bmatrix}
T_{11} & 0 \\
0 & T_{22}
\end{bmatrix}
\begin{pmatrix}
\phi_1^{(n+1)} \\
\phi_2^{(n+1)}
\end{pmatrix} =
\begin{pmatrix}
q_1^{(n)} \\
q_2^{(n)}
\end{pmatrix},
\]

where the right side of the equation is given for:
\[
\begin{pmatrix}
q_1^{(n)} \\
q_2^{(n)}
\end{pmatrix} = -
\begin{bmatrix}
T_{11} & T_{12} \\
T_{21} & T_{22}
\end{bmatrix}
\begin{pmatrix}
\phi_1^{(n)} \\
\phi_2^{(n)}
\end{pmatrix} +
\begin{bmatrix}
R_{11} & R_{12} \\
R_{21} & R_{22}
\end{bmatrix}
\begin{pmatrix}
\phi_1^{(n)} \\
\phi_2^{(n)}
\end{pmatrix} +
\sum_{l=1}^{L} \lambda_l e^{-\lambda_l \Delta t}
\begin{pmatrix}
\xi_l^{(n)} \\
0
\end{pmatrix},
\tag{18}
\]

which is admitted that the neutrons flux in the instant \( n+1 \) is equal to the neutrons flux in the instant \( n \). Assuming that the solution of the equation 17 is given by the following expansion:

\[
\begin{pmatrix}
\phi_1^{(n+1)} \\
\phi_2^{(n+1)}
\end{pmatrix} = \sum_{i=1}^{NP} \alpha_{i,1}^{(n+1)} \begin{pmatrix}
\varphi_{1,i}^{(n+1)} \\
0
\end{pmatrix} + \alpha_{i,2}^{(n+1)} \begin{pmatrix}
0 \\
\varphi_{2,i}^{(n+1)}
\end{pmatrix},
\tag{19}
\]

where \( \varphi_{g,j} \) is the pseudo-harmonic, obtained starting from the following eigenvalues problem

\[
\begin{bmatrix}
T_{gg}
\end{bmatrix}
\begin{pmatrix}
\varphi_{g,j}^{(n+1)}
\end{pmatrix} = \lambda_{g,j}^{(n+1)} \varphi_{g,j}^{(n+1)}
\tag{20}
\]

and substituting the eq. (19) in the eq. (17) and using the eq. (20), is had

\[
\begin{pmatrix}
T_{11} & 0 \\
0 & T_{22}
\end{pmatrix}
\begin{pmatrix}
\phi_1^{(n+1)} \\
\phi_2^{(n+1)}
\end{pmatrix} = \sum_{i=1}^{NP} \alpha_{i,1}^{(n+1)} \begin{pmatrix}
\lambda_{1,i} \varphi_{1,i}^{(n+1)} \\
0
\end{pmatrix} + \alpha_{i,2}^{(n+1)} \begin{pmatrix}
0 \\
\lambda_{2,i} \varphi_{2,i}^{(n+1)}
\end{pmatrix} = \begin{pmatrix}
q_1^{(n)} \\
q_2^{(n)}
\end{pmatrix}.
\tag{21}
\]

Being known that pseudo-harmonics form a orthogonal set, due to the symmetry of the matrix \( [T_{gg}] \), can be written:

\[
\begin{pmatrix}
\varphi_{g,j}^T \\
\varphi_{g,j}
\end{pmatrix}^{(n+1)} \varphi_{g,j}^{(n+1)} = 0, \text{ para } j \neq i,
\tag{22}
\]

and with that multiplying the eq. (21) for \( \varphi_{g,j}^T \) and integrating the resulting equation, be obtained the coefficients of the expansion in (19):

\[
\alpha_{i,g}^{(n+1)} = \frac{\begin{pmatrix}
\varphi_{g,j}^T \\
q_2
\end{pmatrix}^{(n+1)}}{\lambda_{g,j} \begin{pmatrix}
\varphi_{g,j}^T \\
\varphi_{g,j}
\end{pmatrix}^{(n+1)}}, \text{ para } g = 1, 2,
\tag{23}
\]

and consequently the solution of the linear system given in (17) is determined.

To compensate the approach done in the first term on the right side of the eq. 18 a numeric extrapolation is implemented given by
\[
\begin{bmatrix}
0 & T_{12} \\
T_{21} & 0 \\
\end{bmatrix}
\begin{bmatrix}
\phi_1 \\
\phi_2 \\
\end{bmatrix}^{(n)}
\approx
\begin{bmatrix}
0 & T_{12} \\
T_{21} & 0 \\
\end{bmatrix}
\begin{bmatrix}
\phi_1 \\
\phi_2 \\
\end{bmatrix}^{(n)}
+ \gamma
\begin{bmatrix}
0 & T_{12} \\
T_{21} & 0 \\
\end{bmatrix}
\begin{bmatrix}
\phi_1 \\
\phi_2 \\
\end{bmatrix}^{(n-1)}
- \begin{bmatrix}
0 & T_{12} \\
T_{21} & 0 \\
\end{bmatrix}
\begin{bmatrix}
\phi_1 \\
\phi_2 \\
\end{bmatrix}^{(n-2)},
\]

(24)

where \( \gamma \) is an extrapolation factor.

4. RESULTS

To test the proposed method are considered the ANL-BSS-6 [6,7] benchmark and the 2-D TWIGL Seed-Blanket Reactor Benchmark [8]. So much the method proposed as the reference method they were implemented in the programming language Fortran.

4.1. ANL-BSS-6 Benchmark

This benchmark is the problem of slab infinite one-dimensional for transients in spatial kinetics. The geometry consists of three regions according to Fig. 1, whose the nuclear parameters can be found in [6]. O BSS-6 presents two cases different from transients: BSS-6-A1 and BSS-6-A2. In the first case the thermal absorption cross section in the first region is increased linearly in 3% up to 1 s, and maintained constant up to 4 s. In the second case the same absorption cross section is reduced linearly in 1% up to 1 s, and maintained constant up to 4 s.

A mesh of 1 cm was applied in the space discretization, while the size in the step of the adopted time was of 0.001 s.

In the Figs 2 and 3 are presented the comparisons of the present method with the reference method, in the distributions of the neutrons flux, of the fast and thermal group, respectively, in five instants of the transient, for the case BSS-6-A1, both considering Eq. 24, with \( \gamma = 0.98 \). Fig. 4 displays the comparison of the normalized power during the transient for the same case. In this figure is also shown the normalized power obtained by the method proposed without using the extrapolation of Eq. 24, being this indicated by an asterisk. Fig. 5, 6 and 7 show the same comparisons for the case of BSS-6-A2.

Figure 1. 1D Geometry of the ANL-BSS-6 Benchmark Problem
Figure 2. Flux Distribution of the fast group for the ANL-BSS-6-A1 benchmark problem.

Figure 3. Flux Distribution of the thermal group for the ANL-BSS-6-A1 benchmark problem.
Figure 4. Variation of the Normalized Power for the ANL-BSS-6-A1 benchmark problem.

Figure 5. Flux Distribution of the fast group for the ANL-BSS-6-A2 benchmark problem.
Figure 6. Flux Distribution of the thermal group for the ANL-BSS-6-A2 benchmark problem.

Figure 7. Variation of the Normalized Power for the ANL-BSS-6-A2 benchmark problem.
In the case BSS-6-A1 is verified, when comparing the present method with the reference method, that the maximum percentile relative deviation in the neutrons flux is of 16.2%, without the extrapolation (eq. 24), and that the deviation falls for 1.7%, using the (eq. 24), and that both happen in the thermal group. In the case BSS-6-A2 the maximum deviation falls from 26.9% to 1.2% using the extrapolation, and also both happen in the thermal group. In the variation of the normalized power, for the case BSS-6-A1, is observed that the maximum percentile relative deviation is of 7.8%, being reduced to 0.9%, with the extrapolation. In the case BSS-6-A2 this deviation presents the same behavior, falling from 20.4% to 0.9% with the extrapolation.

4.2. 2-D TWIGL Seed-Blanket Reactor Benchmark

This benchmark is a two-dimensional model of a 160 cm square, unreflected seed-blanket reactor using two neutron energy groups and one delayed precursor group. The 2D geometry, with 1/4 symmetry, consists of three regions according to Fig. 8. A complete description of this problem is given in [8]. A mesh of 4 cm was applied in the space discretization, while the size in the step of the adopted time was of 0.001s, and the extrapolation factor $\gamma = 0.95$. The tested transient is initiated by a ramp perturbation, which consists of a 2.3% linear decrease in the thermal absorption cross section of the corner seed assembly (type = 1) over 0.2 seconds. Fig. 9 displays the comparison of the normalized power during the transient. In the case, in the variation of the normalized power, is observed that the maximum percentile relative deviation is of 38%, being reduced to 7.6%, with the extrapolation. Already, in the end of transient, in 5 ms, the percentile relative deviation was of only 0.22%.

![Figure 8. 2D Geometry of the TWIGL Seed-Blanket Reactor Problem](image)
5. CONCLUSIONS

The results generated by the present method have a good accuracy when compared with the reference results, mainly when the suggested extrapolation is applied. The results in the ANL-BSS-6 Benchmark problem had been better of what the results in the 2-D TWIGL Seed-Blanket Reactor Benchmark. In this last case, although to present a maximum percentile relative deviation of 7.6%, the value gotten in the end of the transient for the percentile relative deviation was lesser of what 1%, showing the validity of the considered method.

The authors of this work are developing the present method to simulate problems transients for the geometry three-dimensional in finite differences, as well as for your extension to the existent nodals methods.

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