ONE-DIMENSIONAL MULTIGROUP NEUTRON DIFFUSION EIGENVALUE PROBLEM SOLUTION USING FINITE DIFFERENCE METHOD

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Abstract: In this paper, the solution for a one-dimensional (1D) slab geometry multigroup neutron diffusion eigenvalue problem is achieved by applying the Finite Difference Method (FDM) to discretize the space to solve it numerically. As regards to the formulation of FDM, the problem becomes solving an eigenvalue along with its dominant eigenvector to describe the multiplication factor and the neutron flux distribution vector. Firstly, mathematical basis of neutron diffusion theory applied in 1D problem is established. Discretization of the governing equation with respect to space is described next. The criticality problem of finding the dominant eigenpair is solved by the source iteration (a modified form of power method), which is also explained in the text. After obtaining all the formulation, the calculation is then implemented in MATLAB. The numerical is compared with the analytical solution to verify the fidelity of the proposed method. Good agreement is observed in the comparison; thus, this proposed work can be applied and expanded to more complicated diffusion problems in the future. This work contribution is the primary step to develop a computational tool in nuclear engineering field in Vietnam.

Keywords: *Diffusion, FDM, reactor physics, numerical methods*

I. INTRODUCTION

In reactor physics, surveillance of neutron behavior is main drive in the analysis of the nuclear reactor core. Technically, an essential parameter dominating the physical phenomenon in the core is the neutron distribution in an arbitrary region which can be achieved by solving the neutron transport problem. As an accurate prediction of this distribution can be transferred into the spatial distribution of the reactor power as well as the determination of the slowly time-varying nuclide densities that occur in an operating reactor resulting in the build-up of other fissionable isotopes [1,2]. Mathematically, there are two approaches to solve the neutron transport problem: Deterministic and Stochastic approaches. In terms of the deterministic methods, the diffusion approach is a straightforward method to achieve the neutron flux; however, numerical methods are required for this approach. Many methods have been proposed but the Finite Difference Method [3] (FDM) remains a powerful method due to its transparency and simplicity in implementation. The FDM is used to reduce the partial differential equation into ordinary differential equations, which are organized in form of matrix. As regards to the formulation of FDM, the problem becomes solving an eigenvalue along with its dominant eigenvector to describe the multiplication factor and the neutron flux distribution vector.

This work presents the solution of a one-dimensional (1D) slab geometry multigroup neutron problem using boundary and symmetric conditions. Its purpose is to fulfil the need to acquire a profound knowledge of nuclear reactor physics and to construct a computational tool to solve neutron transport problems in Vietnam, With a good agreement with the analytical solution, this work can be extended into more complicated problems such as in two/three-dimensional (2D/3D) cases by separating the space variables with additional solvers. This paper is organized as follows. A brief mathematical description of the multigroup neutron diffusion theory and the analytical solution for 1D case are established firstly. In the next section, discretization of the governing equation with respect to space is described. The problem of finding the dominant eigenpair of the transport operator is solved by the source iteration (a modified form of power method), which is also explained in the text. After obtaining all the formulation, the calculation is then implemented in MATLAB [4]. The numerical is compared with the analytical solution to verify the fidelity of the proposed method in the Results section. Finally, conclusions and expected future work are presented.

II. MULTIGROUP NEUTRON DIFFUSION THEORY

1. Description of the 1D multigroup neutron diffusion equation

In this section, the equation governing the modeling of the neutron diffusion are briefly presented. In an energy group g, the time independent equation with Fick's Law [2] approximation is given as:

$$\frac{d}{dx}\underbrace{J_g(x)}_{-D_g(x)\frac{d}{dx}\phi_g(x)} + \Sigma_{r,g}(x)\phi(x) = \sum_{\substack{g'=1\\g'\neq g}}^{G} \Sigma_{g'g}(x)\phi_{g'}(x) + \frac{\chi_g}{k_{eff}}\sum_{g'=1}^{G} \nu\Sigma_{f,g'}(x)\phi_{g'}(x), \quad (1)$$

where the notations are defined as follows.

- g: the energy group index,
- D_g: diffusion constant (cm),
- $\Sigma_{r,g}$: macroscopic removal cross section (cm^{-1}),
- $\Sigma_{gg'}$: macroscopic scattering cross section from group $g'$to group g (cm^{-1}),
- $\Sigma_{f,g'}$: macroscopic fission cross section (cm^{-1}),
- ν: the average number of neutrons emitted per fission induced in group g;
- χ_g: fission spectrum normalized as $\sum_{g=1}^{G}\chi_g = 1$,
- ϕ_g: neutron flux (cm^{-2}sec^{-1}),
- k_{eff}: effective multiplication factor, $g = 1,2, \dots G$.

Please note that, in above equation, for the sake of diffusion approximation, the dependence of angle in all terms is neglectable. With the assumption that the medium is homogeneous, .i.e. the space dependence for parameters can be ignored. The final form of the 1D neutron diffusion equation is:

$$-D_g\frac{d^2}{dx^2}\phi_g(x) + \Sigma_{r,g}\phi_g(x) = \sum_{\substack{g'=1\\g'\neq g}}^{G} \Sigma_{g'g}\phi_{g'}(x) + \frac{\chi_g}{k_{eff}}\sum_{g'=1}^{G} \nu\Sigma_{f,g'}\phi_{g'}(x). \quad (2)$$

The analytical solution for the equation (2) is described in the next section.

2. Analytical solution for the 1D slab geometry multigroup neutron diffusion problem

For the sake of simplicity, here we use two groups of energy, i.e. thermal and fast neutron group. One can later apply the same process into a higher number of groups depending on his own interest. Firstly, equation (2) needs transforming into solvable form by applying *Laplacian* and rewrite in terms of matrix:

$$\begin{bmatrix} -D_1\nabla^2 + \Sigma_{r,1} & 0 \\ -\Sigma_{12} & -D_2\nabla^2 + \Sigma_{r,2} \end{bmatrix} \cdot \begin{bmatrix} \phi_1(x) \\ \phi_2(x) \end{bmatrix} = \frac{1}{k_{eff}} \begin{bmatrix} \nu\Sigma_{f,1} & \nu\Sigma_{f,2} \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \phi_1(x) \\ \phi_2(x) \end{bmatrix}. \quad (3)$$

As can be seen from equation (3), the up-scattering term from thermal group to fast group is not considered [5]. The neutron flux for both thermal and fast groups are the solution of partial differential equations of the elliptic type when the time dependency is ignored. Accordingly, the Helmholtz's equation is satisfied for group g as [1, 2]:

$$\nabla^2\phi_g(x) + B^2\phi_g(x) = 0, \tag{4}$$

with B^2 is the geometry buckling parameter. Please note the subscript g for the geometry buckling has been removed to not confuse it with the group index. By combining this condition to equation (3) yields:

$$\begin{bmatrix} D_1B^2 + \Sigma_{r,1} & 0 \\ -\Sigma_{12} & D_2B^2 + \Sigma_{r,2} \end{bmatrix} \cdot \begin{bmatrix} \phi_1(x) \\ \phi_2(x) \end{bmatrix} = \frac{1}{k_{eff}} \begin{bmatrix} \nu\Sigma_{f,1} & \nu\Sigma_{f,2} \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \phi_1(x) \\ \phi_2(x) \end{bmatrix}. \tag{5}$$

Algebraically, in order to solve equation (5), the determinant of the coefficient matrix must be zero. This condition resulted in a quadratic equation:

$$(B^2)^2 + 2bB^2 + c = 0, \tag{6}$$

with $b = \frac{1}{2}\left(\frac{\Sigma_{r,1}}{D_1} + \frac{\Sigma_{r,2}}{D_2} - \frac{\nu\Sigma_{f,1}}{D_1k_{eff}}\right)$ and $c = \left(\frac{\Sigma_{r,1}\Sigma_{r,2}}{D_1D_2}\right) - \frac{1}{k_{eff}}\left(\frac{(\nu\Sigma_{f,1}\Sigma_{r,2}+\nu\Sigma_{f,2}\Sigma_{12})}{D_1D_2}\right)$.

One can easily notice that the term $b^2 - c$ is always positive due to its only dependency on the nuclear data parameters. Thus equation (6) always has distinct solutions. After defining the buckling parameter, attempt to solve the diffusion equation is introduced. With the assumption of exponential shape in the neutron flux in both thermal and fast region, the general solution for the thermal flux is illustrated as:

$$\phi_2(x) = C_1\cos(Bx) + C_2\sin(Bx)\,. \tag{7}$$

By substituting ϕ_2 into equation (5), the fast flux is given:

$$\phi_1(x) = \frac{(-D_2\nabla^2 + \Sigma_{r,2})}{\Sigma_{21}}(C_1\cos(Bx) + C_2\sin(Bx)). \tag{8}$$

To determine the flux within this reactor, above equations must be solved subject to the boundary conditions (BCs) that flux vanishes at the extrapolated faces of the slab geometry illustrated in figure 1, i.e.:

$$\phi_g\left(\frac{\widetilde{H}_g}{2}\right) = \phi_g\left(-\frac{\widetilde{H}_g}{2}\right) = 0, \tag{9}$$

where: $\widetilde{H}_g = H + 2d_g, d_g = 2.13D_g$

Due to the symmetry of this problem, there can be no net flow of neutrons at the center of the plane. Since the neutron current density is proportional to the derivative of flux, this means that:

$$\frac{d\phi_g(x)}{dx} = 0, x = 0 \leftrightarrow \phi_g(-x) = \phi_g(x). \tag{10}$$

Under those BCs, a system of unknowns can be solved to achieve coefficient C_i to express the neutron flux. Hence, for the thermal group, in such conditions ($\widetilde{H}_2 \cong H$):

$$C_1 = 0;\ B = \frac{n\pi}{H}(n\ is\ an\ even\ number);\ C_2 = 0; B = \frac{n\pi}{H}(n\ is\ an\ odd\ number) \tag{11}$$

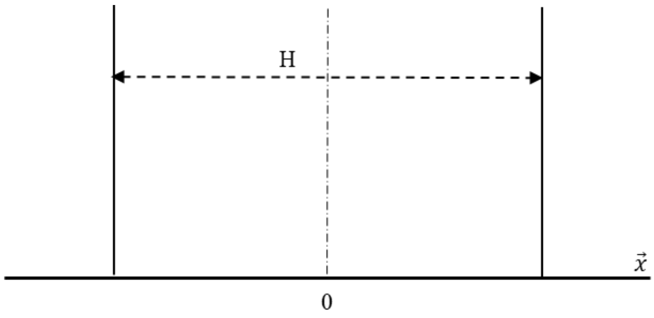

Figure 1. Slab reactor geometry

This is satisfied if B assumes any of the values B_n, where:

$$B_n = \frac{n\pi}{H}\ (n = 1, \dots . \infty). \tag{12}$$

After getting the value of buckling, the multiplication factor k_{eff} now can be obtained, which will yield a nontrivial solution of the equation (5):

$$k_{eff} = \frac{\left(\nu\Sigma_{f,2}\Sigma_{12} + \nu\Sigma_{f,1}\left(D_2 B_n^2 + \Sigma_{r,2}\right)\right)}{\left(D_1 B_n^2 + \Sigma_{r,1}\right) \times \left(D_2 + \Sigma_{r,2}\right)}. \tag{13}$$

For the fundamental mode solution, n = 1 associated with the eigenfunction shown as Equation 14. After obtaining the analytical solution of the neutron flux, the discretization in space applied in the FDM is presented in the next section.

$$B = \frac{\pi}{H}\ ;\ \phi_2(x) = \cos\left(\frac{\pi}{H}x\right);\ \phi_1(x) = \frac{\left(D_2\left(\frac{\pi}{H}\right)^2 + \Sigma_{r,2}\right)}{\Sigma_{12}}\left(\cos\left(\frac{\pi}{H}x\right)\right). \tag{14}$$

III. SPACE DISCRETIZATION OF NEUTRON BALANCE EQUATION

In this section, the formulation of FDM applied for the neutron flux is first presented. After the matrix form of the discrete equation, the inverse power method approach to achieve the fundamental mode is illustrated.

1. Formulation of FDM applied in diffusion equation based on box-scheme

The first step in developing a numerical solution procedure is to replace the continuous spatial dependence of the flux, with the values of the average flux at discrete spatial meshes. Therefore, numerically, the neutron flux can be obtained as long as the number of meshes is large enough [6]. One can note that the finite different discretized equations solution is equivalent to the differential equation if only the mesh size approach null. In this 1D problem, we subdivide the interval $0 \le x \le H$ of interest into I subintervals of length $h = \frac{H}{I}$. Based on the box scheme discretization [7], let's integrate equation (1) over the node and divide by the node length h yields:

$$\int_0^1 \left[\frac{d}{d\mathcal{E}} J_g^k + \Sigma_{r,g}^k \phi_g^k\right] d\mathcal{E} = \int_0^1 \left[\frac{1}{k_{eff}} \chi_g^k \sum_{g'=1}^{G} \nu\Sigma_{f,g'}^k \phi_g^k + \sum_{\substack{g'=1 \\ g' \neq g}}^{G} \Sigma_{g'g}^k \phi_{g'}^k\right] d\mathcal{E}, \tag{15}$$

with $\mathcal{E} = \frac{x}{h} \leftrightarrow dx = hd\mathcal{E}$ and $\Sigma_{r,g}^k = \Sigma_{t,g}^k - \Sigma_{gg}^k$.

Using the definition of the neutron current J [2], the leakage term in node k can be expressed as:

$$\int_{x_k-\frac{h}{2}}^{x_k+\frac{h}{2}} dx\left(\frac{d}{dx}D_g(x)\frac{d\phi_g}{dx}\right) \approx D_g\frac{d\phi_g}{dx}|_{x_k+\frac{h}{2}} - D_g\frac{d\phi_g}{dx}|_{x_k-\frac{h}{2}}$$
$$= \frac{1}{2}\left(D_g^k + D_g^{k+1}\right)\frac{\left(\phi_g^{k+1} - \phi_g^k\right)}{h} - \frac{1}{2}\left(D_g^{k-1} + D_g^k\right)\frac{\left(\phi_g^k - \phi_g^{k-1}\right)}{h} \tag{16}$$

Therefore, the general form of the neutron balance at node k is given as:

$$-\widetilde{D}_g^{k-1}\phi_g^{k-1} + \left(\widetilde{D}_g^{k-1} + \widetilde{D}_g^k + \Sigma_{r,g}^k h\right)\phi_g^k - \widetilde{D}_g^k\phi_g^{k+1} = S_g^k, \tag{17}$$

where:

$$\begin{cases} \widetilde{D}_g^{k-1} = \dfrac{2\beta_g^{k-1}\beta_g^k}{\beta_g^k + \beta_g^{k-1}}, \widetilde{D}_g^k = \dfrac{2\beta_g^k\beta_g^{k+1}}{\beta_g^k + \beta_g^{k+1}}, \beta_g^k = \dfrac{D_g^k}{h} \\ S_g^k = h\left(\dfrac{1}{k_{eff}}\chi_g^k\displaystyle\sum_{g'=1}^{G}\nu\Sigma_{f,g'}^k\phi_g^k + + \sum_{\substack{g'=1\\g'\neq g}}^{G}\Sigma_{g'g}^k\phi_{g'}^k\right) \end{cases} \tag{17}$$

Now the boundary conditions (BC) must be considered. Using the albedo boundary condition [8] which generally expressed as:

$$\begin{cases} Left\ BC\text{: } J_g^0 = -\alpha_L\phi_g^0 \\ Right\ BC\text{: } J_g^{I+1} = -\alpha_R\phi_g^{I+1} \end{cases}, with\ \alpha = \begin{cases} \infty, flux\ zero \\ 0, net\ current\ zero \\ 0.5, incoming\ partial\ current\ zero \end{cases} \tag{18}$$

Then the balance equation at the left and right BC are:

$$\left(\widetilde{D}_g^0 + \widetilde{D}_g^1 + \Sigma_{r,g}^1 h\right)\phi_g^1 - \widetilde{D}_g^1\phi_g^2 = S_g^1, \tag{19}$$

$$-\widetilde{D}_g^{I-1}\phi_g^{I-1} + \left(\widetilde{D}_g^{I-1} + \widetilde{D}_g^I + \Sigma_{r,g}^I h\right)\phi_g^I = S_g^I. \tag{20}$$

Combining equation (17), (19), (20) the discretized 1D multigroup neutron diffusion equation at node k is displayed as in equation (21):

$$-l_g^k\phi_g^{k-1} + d_g^k\phi_g^k - u_g^k\phi_g^{k+1} = S_g^k = \frac{1}{k_{eff}}\chi_g^k \underbrace{h\sum_{g'=1}^{G}\nu\Sigma_{f,g'}^k\phi_g^k}_{\psi^k} + h\sum_{\substack{g'=1\\g'\neq g}}^{G}\Sigma_{g'g}^k\phi_{g'}^k$$
$$\leftrightarrow -l_g^k\phi_g^{k-1} + d_g^k\phi_g^k - u_g^k\phi_g^{k+1} - h\sum_{\substack{g'=1\\g'\neq g}}^{G}\Sigma_{g'g}^k\phi_{g'}^k = \frac{1}{k_{eff}}\chi_g^k\psi^k \tag{21}$$

with:

$$l_g^k = \widetilde{D}_g^{k-1};\ u_g^k = \widetilde{D}_g^k;\ d_g^k = l_g^k + u_g^k + h\Sigma_{r,g}^k \tag{22}$$

Therefore, all the nodes in the problem can be expressed in matrix form as:

$$M\phi = \frac{1}{k_{eff}} F\phi \tag{23}$$

where:

$$M = \begin{bmatrix} D_1 & U_1 & 0 & \cdots & 0 \\ L_2 & D_2 & U_2 & \cdots & 0 \\ 0 & \ddots & \ddots & \ddots & 0 \\ 0 & 0 & L_{I-1} & D_{I-1} & U_{I-1} \\ 0 & 0 & \cdots & L_I & D_I \end{bmatrix}, D_k = \begin{bmatrix} d_1^k & 0 & & \\ -h\Sigma_{12}^k & d_2^k & & \\ & & \ddots & \\ -h\Sigma_{1G}^k & \cdots & -h\Sigma_{G-1,G}^k & d_G^k \end{bmatrix}$$

$$L_k = \begin{bmatrix} -l_1^k & 0 & & 0 \\ 0 & \ddots & 0 & \\ & 0 & -l_{G-1}^k & 0 \\ 0 & & 0 & -l_G^k \end{bmatrix}, U_k = \begin{bmatrix} -u_1^k & 0 & & 0 \\ 0 & \ddots & 0 & \\ & 0 & -u_{G-1}^k & 0 \\ 0 & & 0 & -u_G^k \end{bmatrix} \tag{24}$$

$$\phi = \left[\left[\phi_g^1\ \phi_{g+1}^1 \dots \phi_G^1\right]\left[\phi_g^2\ \phi_{g+1}^2 \dots \phi_G^2\right] \dots \left[\phi_g^I\ \phi_{g+1}^I \dots \phi_G^I\right]\right]^T$$

$$F = \begin{bmatrix} F^1 & 0 & & & 0 \\ 0 & \ddots & 0 & & \\ & 0 & F^k & 0 & \\ & & 0 & \ddots & 0 \\ 0 & & & 0 & F^I \end{bmatrix}, F^k = h\begin{bmatrix} \chi_1^k \nu\Sigma_{f1}^k & \cdots & \chi_1^k \nu\Sigma_{fg}^k & \cdots & \chi_1^k \nu\Sigma_{fG}^k \\ \chi_2^k \nu\Sigma_{f1}^k & \cdots & \chi_2^k \nu\Sigma_{fg}^k & \cdots & \chi_2^k \nu\Sigma_{fG}^k \\ \vdots & & \vdots & & \vdots \\ \chi_{g'}^k \nu\Sigma_{f1}^k & \cdots & \chi_{g'}^k \nu\Sigma_{fg}^k & \cdots & \chi_{g'}^k \nu\Sigma_{fG}^k \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

As shown in equation (23), the problem now becomes solving the eigenvalue problem as:

$$k_{eff}\phi = M^{-1}F\phi \leftrightarrow \left(M^{-1}F - k_{eff}I\right)\phi = 0. \tag{25}$$

Thus, to satisfy equation (25) in the fundamental mode, ϕ is an eigenvector associated with the dominant eigenvalue k_{eff}. Applying the eigenvalue iteration method [6, 7, 8] for outer iteration and Jacobi method [9] to solve the linear system $Ax = b$, the iteration scheme to achieve ϕ and k_{eff} is given in figure 2.

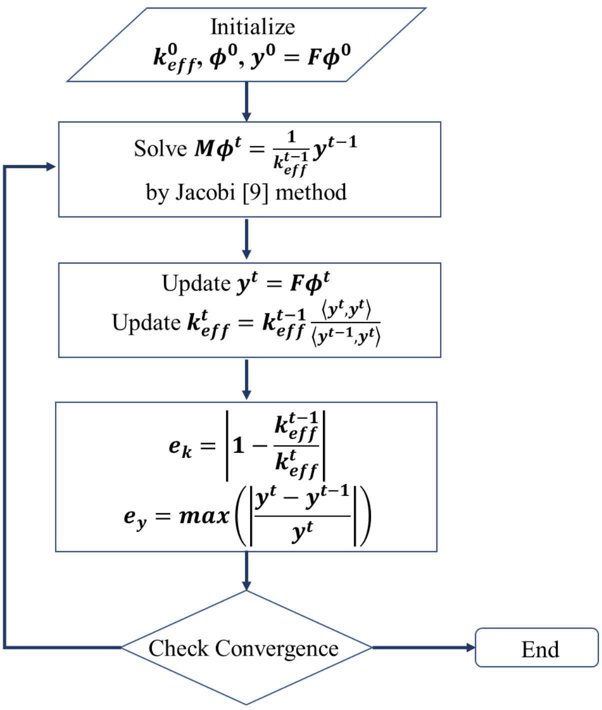

Figure 2. Iteration scheme to calculate k_{eff} and ϕ

IV. RESULTS AND DISCUSSION

After obtaining all the formulation of the discretized equation, a MATLAB [4] script is written to perform the calculation. This section presents the result for a homogenous bare slab reactor. Finally, the conclusion and discussion are drawn in the end of this section.

1. Result of homogeneous bare slab reactor

The results obtained in both analytical solution and numerical solution for the neutron diffusion equation have been compared in this sub-section. Table I displays the nuclear data used in the homogeneous slab reactor with the size of 40cm. In the calculation process, the solver includes outer iteration and inner iteration using Jacobi method [9] as shown in Figure 2. With the convergence criteria is 10^{-5}, Figure 3 and 4 illustrate the distribution of multigroup neutron flux and the fission source. In addition, the multiplication factor k_{eff} is compared between FDM and analytical solution given in equation (13) illustrating in Table II. The simulation for this simple problem with 100 FDM nodes and two groups of energy requires 0.142 seconds.

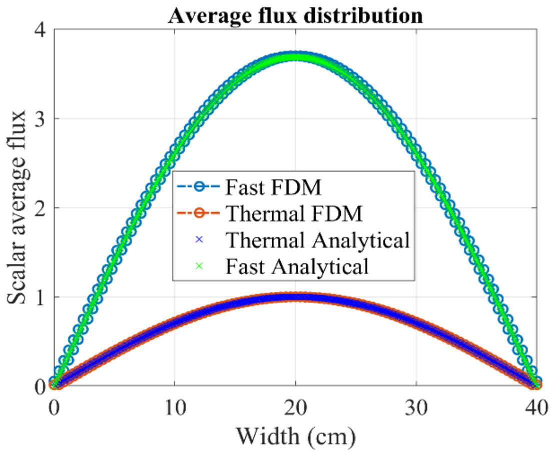

Figure 3. Average flux distribution

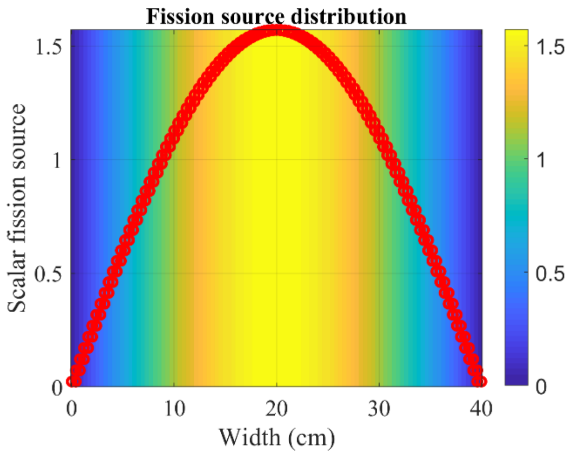

Figure 4. Fission source distribution

As illustrated, the results from FDM agrees very well with the analytical solution. In terms of the multiplication factor k_{eff}, only 2 pcm is observed. One may realize that using a large number of node leads to tht

Table 1. Group constants used in homogeneous slab reactor [7]

Group	$\nu\Sigma_f$	Σ_r	$\Sigma_{gg'}$	D
1	5.32328E-03	2.61000E-02	1.74514E-2	1.436040
2	9.52684E-02	6.20800E-02	1.25211E-3	0.398363

Table II. Comparison of multiplication factor between FDM and equation (5)

Multiplication factor	Analytical	FDM
k_{eff}	0.8977743	0.8977955

2. Conclusion and Discussion

The objective of this work was verified and obtained. The FDM solver script can be applied to 1D geometry multigroup slab reactor and generate the multiplication factor as well as the flux distribution. In our 1D simple case, using the mesh size of 0.4 cm in 100 nodes, it requires around 8 iterations to achieve the convergence after 0.142 seconds. In the iteration process, we also applied the Wielandt Shift [10] to predict the dominant ratio to accelerate the convergence speed of both fission source and the multiplication factor. In this work, only homogeneous case was considered, however, using the similar spacing discretization scheme, it can be expanded to heterogeneous case, which presents the reflector in the reactor. Furthermore, by applying same process in each direction, this work can also work for 3D cases. The only drawback of FDM is its extensive computational resources requirement to achieve a good accuracy because the mesh size must be smaller than the thermal diffusion length. As a result, in a practical problem, to achieve a fair fidelity, FDM code must use 106 meshes for all directions, thus it is not good to bear such a burden. In the future development of simulation code, advanced numerical methods will be applied and coupled with the FDM solver, particularly, the transverse integrated nodal method (TINM) [1, 2] will be the candidate for our implementation.

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GIẢI BÀI TOÁN TRỊ RIÊNG TRONG KHUẾCH TÁN NEUTRON MỘT CHIỀU ĐA NHÓM SỬ DỤNG PHƯƠNG PHÁP SAI PHÂN HỮU HẠN

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Tóm tắt nội dung: Trong nghiên cứu này, lời giải cho bài toán khuếch toán neutron một chiều đa nhóm được tính toán dựa trên phương pháp sai phân hữu hạn (FDM). Trong quá trình hình thành các hệ phương trình sử dụng trong FDM, bài toán khuếch tán neutron trở thành bài toán tính trị riêng lớn nhất và vector trị riêng tương ứng để diễn tả hệ số nhân neutron và phân bố thông lương neutron. Đầu tiên, các mô hình toán cơ bản áp dụng trong bài toán khuếch tán một chiều được trình bày, Tiếp theo là phần chia nhỏ bài toán theo không gian để hình thành hệ phương trình cho FDM. Sau đó là việc tính toán tới hạn để tìm cặp trị riêng và vector trị riêng giải bằng phương pháp lặp nguồn được trình bày chi tiết trong bài viết này. Sau khi hình thành được hệ thống các phương trình, việc triển khai thực hiện tính toán được dựa trên phần mềm MATLAB. Các kết quả tính toán bằng phương pháp số được so sánh với phương pháp giải tích để đành giá tính tin cậy của phương pháp. Với sai số gần như là không đáng kể, cách giải để xuất này có thể áp dụng cho các bài toán khuếc tán phức tạp hơn trong tương lai. Nghiên cứu này là bước khởi đầu trong việc xây dựng công cụ tính toán lò phản ứng trong cũng như hỗ trợ pháp triển ngành kỹ thuật hạt nhân ở Việt Nam.

Từ khóa: *Phương trình khuếch tán, FDM, vật lý lò phản ứng, phương pháp số*