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Analytical solution of the multigroup neutron diffusion equation coupled with an iterative method

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ABSTRACT

Many numerical methods are being used to solve the multigroup neutron diffusion equation for different types of nuclear reactors. These methods solve this equation quite accurately and determine the neutron flux and power distribution in the reactor as well as the eigenvalue of the reactor core. In this paper, we are proposing the integration of an analytical solution with an iterative method to determine the neutron flux distribution in the reactor and the effective eigenvalue. To do this, we solve the one-dimensional neutron diffusion equation for two energy groups, where the nuclear parameters are uniform in both nuclear fuel and reflector regions. The eigenvalue will be determined from the analytical solution using the power method iteratively until reaching convergence in both flux and eigenvalue. The results obtained in this paper are compared to those from numerical methods used to validate the proposed method.

Keywords: **Neutron diffusion equation, analytical solution, iterative method, eigenvalue, slab reactor.**

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1. INTRODUCTION

Aiming to describe different types of practical problems as well experimental tests, many algorithms have been developed seeking numerical results to model different types of problems from different areas of knowledge. Thus, there are different types of numerical methods, of which we highlight solution with iterative methods [1]. These methods consist of taking an initial value and after successive calculations, the results converge to the solution of the problem. In these calculations, the convergence is specified to decide when a solution was found sufficiently precise. One of the major factors that contribute to this is the ability to implement computer codes and their relationship to the different areas of knowledge: physics, engineering, mathematics and others, as well as the ease of modeling quite complex problems, especially when analytical solutions are not easily found or even non-existent. As an example, we can mention the neutron transport equation [2] which is an integro-differential equation with seven independent variables describing the distribution of neutrons in the nuclear reactor.

In this paper, we present an analytical solution for the neutron flux by solving the one-dimensional neutron diffusion equation for two energy groups using boundary conditions, along with neutron flux and current continuity. This solution is also coupled with an iterative method to determine the effective eigenvalue of the system and its respective neutron flux distribution in the reactor. In these calculations, the results obtained are compared with the results of numerical methods to validate the proposed method.

One of the greatest advantages of using an analytical solution is to obtain an expression for the neutron flux in regions where nuclear parameters are homogeneous. Thus, we need to solve the neutron diffusion equation in each homogeneous region, and by imposing flux and current continuity, we couple all the different regions that make up the reactor. It is worth noting that the analytical solution is valid throughout homogeneous region and does not depend on the region size. However, if we use the finite difference method [1], the validity of this method consists in having a smaller calculation region or equal to the diffusion length, such that $L_g^n \le \sqrt{\frac{D_g^n}{\Sigma_{ag}^n}}$ where D_g^n and Σ_{ag}^n are, respectively, the diffusion coefficient and the macroscopic absorption cross section of the region *n* and energy group *g*. With this, the number of regions to be used in the calculations increases significantly, increasing the computational effort to solve very simple problems.

2. ONE-DIMENSIONAL NEUTRON DIFFUSION EQUATION WITH TWO ENERGY GROUPS

All the development of reactors theory is related to the production of neutrons in the core; with this, the projects developed for nuclear reactors are designed to sustain and stabilize the reactions of nuclear fission in the core. This balance of neutrons is obtained according to the number of neutrons that are produced and removed from the reactor. To accompany the multiplication of neutrons in the core, we use the neutron continuity equation and Fick's law [2], which, for the one-dimensional case with two energy groups and independent of time, are expressed by the following equations, respectively

$$\frac{d}{dx}J_g(x) + \Sigma_{rg}(x)\phi_g(x) = \sum_{\substack{g'=1 \\ g'\neq g}}^{2} \Sigma_{gg'}(x)\phi_{g'}(x) + \frac{\chi_g}{k_{eff}}\sum_{g'=1}^{2} \nu\Sigma_{fg'}(x)\phi_{g'}(x), \tag{1}$$

and

$$J_g(x) = -D_g(x)\frac{d}{dx}\phi_g(x). \tag{2}$$

Substituting Eq.(2) into (1), we obtain the neutron diffusion equation [3], defined to an eigenvalue problem and expressed only in terms of the neutron flux, such that,

$$-\frac{d}{dx}\left(D_g(x)\frac{d}{dx}\phi_g(x)\right) + \Sigma_{rg}(x)\phi_g(x) = \sum_{\substack{g'=1 \\ g'\neq g}}^{2} \Sigma_{gg'}(x)\phi_{g'}(x) + \frac{\chi_g}{k_{eff}}\sum_{g'=1}^{2} \nu\Sigma_{fg'}(x)\phi_{g'}(x), \tag{3}$$

where $D_g(x)$ is the diffusion coefficient of the group *g*, $\Sigma_{rg}(x)$ is the macroscopic removal cross section of the group *g*, $\Sigma_{gg'}(x)$ is the macroscopic scattering cross section of group *g'* for the group *g*, $\nu\Sigma_{fg'}(x)$ is the product of the average number of neutrons emitted by fission and the macroscopic fission cross section of group *g'*, χ_g is the fission spectrum of the group *g*, $\phi_g(x)$ is the neutron flux of the group *g* at position *x* in the reactor core and k_{eff} is the effective eigenvalue.

Due to the reactor being homogeneous in the case of one single region, or homogeneous by regions in the case of fuels and reflectors regions, the nuclear parameters are uniform within each region *n*. In others words, $D_g(x) = D_g^n$, $\Sigma_{rg}(x) = \Sigma_{rg}^n$, $\Sigma_{gg'}(x) = \Sigma_{gg'}^n$ and $\nu\Sigma_{fg'}(x) = \nu\Sigma_{fg'}^n$. Thus, Eq.(3) is

$$-D_g^n \frac{d^2}{dx^2}\phi_g(x) + \Sigma_{rg}^n \phi_g(x) = \sum_{\substack{g'=1 \\ g' \neq g}}^{2} \Sigma_{gg'}^n \phi_{g'}(x) + \frac{\chi_g}{k_{eff}} \sum_{g'=1}^{2} \nu\Sigma_{fg'}^n \phi_{g'}(x). \tag{4}$$

We shall seek to solve Eq.(4) analytically for different regions, such as nuclear fuels and neutron reflectors.

2.1. Analytical solution of the neutron diffusion equation for fuel regions

The neutron diffusion equation, given by Eq.(4) for two energy groups, can be written as follows:

$$-D_1^n \frac{d^2}{dx^2}\phi_1(x) + \Sigma_{r1}^n \phi_1(x) = \frac{1}{k_{eff}}\left(\nu\Sigma_{f1}^n \phi_1(x) + \nu\Sigma_{f2}^n \phi_2(x)\right), \tag{5}$$

and

$$-D_2^n \frac{d^2}{dx^2}\phi_2(x) + \Sigma_{r2}^n \phi_2(x) = \Sigma_{21}^n \phi_1(x), \tag{6}$$

where $\phi_1(x)$ and $\phi_2(x)$ represent, respectively, the fast and thermal neutron flux. Note that we are not considering up-scattering.

The Helmholtz equation [4] for a multigroup structure g, is given by:

$$\nabla^2\phi_g(x) + B^2\phi_g(x) = 0, \qquad g = 1,2 \tag{7}$$

where B^2 will define the type of function to be employed in the solution of Eq.(7), such that if B^2 is positive, we will have trigonometric functions. If B^2 is negative, we will have hyperbolic or exponential functions. Substituting Eq.(7) in (5) and (6), we have

$$\begin{bmatrix} D_1^n B^2 + \Sigma_{r1}^n - \frac{1}{k_{eff}}\nu\Sigma_{f1}^n & -\frac{1}{k_{eff}}\nu\Sigma_{f2}^n \\ -\Sigma_{21}^n & D_2^n B^2 + \Sigma_{r2}^n \end{bmatrix} \cdot \begin{bmatrix} \phi_1(x) \\ \phi_2(x) \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}. \tag{8}$$

In order for the equation to have non-trivial solutions, the determinant of this matrix must be zero, resulting in:

$$(D_1^n B^2 + \Sigma_{r1}^n - \frac{1}{k_{eff}}\nu\Sigma_{f1}^n)(D_2^n B^2 + \Sigma_{r2}^n) - \frac{1}{k_{eff}}\nu\Sigma_{f2}^n\Sigma_{21}^n = 0, \tag{9}$$

of which we have,

$$\left(B^2\right)^2 + \left(\frac{\Sigma_{r1}^n}{D_1^n} + \frac{\Sigma_{r2}^n}{D_2^n} - \frac{1}{k_{eff}}\frac{\nu\Sigma_{f1}^n}{D_1^n}\right)B^2 + (1 - \frac{k_\infty}{k_{eff}})\frac{\Sigma_{r1}^n\Sigma_{r2}^n}{D_1^n D_2^n} = 0, \tag{10}$$

where k_∞ is obtained by neglecting the leakage term in Eq.(4) and is given by

$$k_\infty = \frac{\nu\Sigma_{f1}^n\Sigma_{r2}^n + \nu\Sigma_{f2}^n\Sigma_{21}^n}{\Sigma_{r1}^n\Sigma_{r2}^n}. \tag{11}$$

Defining $w \equiv B^2$, Eq.(10) expressed as follows

$$w^2 + \left(\frac{\Sigma_{r1}^n}{D_1^n} + \frac{\Sigma_{r2}^n}{D_2^n} - \frac{1}{k_{eff}}\frac{\nu\Sigma_{f1}^n}{D_1^n}\right)w + (1 - \frac{k_\infty}{k_{eff}})\frac{\Sigma_{r1}^n\Sigma_{r2}^n}{D_1^n D_2^n} = 0, \tag{12}$$

of which we have as a solution,

$$w_1 = \frac{b}{2}\left(-1+\sqrt{1-\frac{4c}{b^2}}\right), \tag{13}$$

and

$$w_2 = \frac{b}{2}\left(-1-\sqrt{1-\frac{4c}{b^2}}\right), \tag{14}$$

with $b = \frac{\Sigma_{r1}^n}{D_1^n} + \frac{\Sigma_{r2}^n}{D_2^n} - \frac{1}{k_{eff}}\frac{\nu\Sigma_{f1}^n}{D_1^n}$ and $c = (1-\frac{k_\infty}{k_{eff}})\frac{\Sigma_{r1}^n\Sigma_{r2}^n}{D_1^n D_2^n}$.

Since we defined the values w in function of B^2, we have these parameters, $w's$, define the type of solution for the neutron diffusion equation, i.e., trigonometric functions for $w_g > 0$ and hyperbolic or exponential functions for $w_g < 0$. The B values used in the arguments of these functions will be given by: $B_g = \pm\sqrt{|w_g|}$.

Since the equation is bi-square, we have a solution with four coefficients to be determined, so we need four boundary conditions to determine these coefficients. The values w_g change depending on the eigenvalue problem and the type of region. As our goal is to solve Eq.(4) iteratively using the power method [1], the values of w_g will change every iterative process, so that the neutron flux is expressed as a combination of trigonometric and hyperbolic or exponential functions.

From the values of w_g, we can write an expression for the neutron flux. To illustrate, suppose w_1 is positive and w_2 is negative. Therefore, the thermal neutron flux may be expressed as follows,

$$\phi_2(x) = c_1\sin(B_1x) + c_2\cos(B_1x) + c_3\sinh(B_2x) + c_4\cosh(B_2x). \tag{15}$$

Due to the system to be coupled, as shown in Eqs.(5) and (6), the solution to the fast flux can be obtained by substituting Eq.(15) in (6), which we have

$$\phi_1(x) = \frac{\Sigma_{r2}^n + D_2^n B_1^2}{\Sigma_{21}^n}(c_1 \sin(B_1 x) + c_2 \cos(B_1 x)) + \frac{\Sigma_{r2}^n - D_2^n B_2^2}{\Sigma_{21}^n}(c_3 \sinh(B_2 x) + c_4 \cosh(B_2 x)). \quad (16)$$

Using flux and current continuity conditions and boundary conditions, we can determine the coefficients c_i of Eqs.(15) and (16) and thus obtain the neutron flux distribution in the reactor. Note that these coefficients do not depend on the energy group and are the same for both thermal and fast flux.

2.2. Analytical solution of the neutron diffusion equation for reflector regions

For the reflector region, the neutron diffusion equation undergoes some changes both in the nuclear parameters as in its functional form, since for this region there is no neutron fission. This is due to the fact that the main objective of the neutron reflectors is to minimize the neutron leakage, making the neutrons return to the reactor core to generate new fissions, besides contributing to the economy of fuel elements [2]. Therefore, this equation is written as follows:

$$-D_1^n \frac{d^2}{dx^2}\psi_1(x) + \Sigma_{r1}^n \psi_1(x) = 0, \quad (17)$$

and

$$-D_2^n \frac{d^2}{dx^2}\psi_2(x) + \Sigma_{r2}^n \psi_2(x) = \Sigma_{21}^n \psi_1(x). \quad (18)$$

The solution of the neutron diffusion equation for fast and thermal group, in the reflector region, are respectively,

$$\psi_1(x) = r_1 e^{x/L_1^n} + r_2 e^{-x/L_1^n}, \quad (19)$$

and

$$\psi_2(x) = \left(\frac{D_1^n \Sigma_{21}^n}{\Sigma_{r2}^n D_1^n - \Sigma_{r1}^n D_2^n}\right)\left(r_1 e^{x/L_1^n} + r_2 e^{-x/L_1^n}\right) + r_3 e^{x/L_2^n} + r_4 e^{-x/L_2^n}, \quad (20)$$

where $L_1^n = \sqrt{\frac{D_1^n}{\Sigma_{r1}^n}}$ and $L_2^n = \sqrt{\frac{D_2^n}{\Sigma_{r2}^n}}$ are the respective diffusion length of the fast and thermal group.

Eqs.(19) and (20) represent solutions for the neutron flux in the reflector region, while Eqs.(15) and (16) represent solutions for the neutron flux in the fuel regions. Note that Eq.(19) is decoupled from Eq.(20), so if we impose boundary and continuity conditions, we determine only the coefficients r_1 and r_2. Now, using Eq.(20) we can determine all the coefficients.

Once the solutions for the neutron flux in the fuel and reflector regions are known, we can use the power method [1] to determine the eigenvalue in function of the neutron flux through iterative processes.

3. RESULTS AND DISCUSSION

We present the results obtained by the analytical solution of the neutron diffusion equation in a slab reactor for two energy groups and compare the results from the Nodal Expansion Method (NEM) [5]. To use the power method for calculating the eigenvalue, we need to calculate the average values of the flux in each fuel region. For this, we solve the following cases.

3.1. Fuel regions

The solution of the neutron diffusion equation for nuclear fuel regions are given by Eqs.(15) and (16). As can be seen, we need four boundary and continuity conditions for each region to determine the coefficients for the neutron flux. For simplicity, we will adopt the following notations for both the neutron flux $\phi_g^n(\mathrm{x})$, and current $J_g^n(\mathrm{x})$, where the indices *n* and *g* denote, respectively, regions and energy groups. Those conditions are:

i) Null net current in the origin for the thermal group: $J_2^1(0) = 0$;

ii) Current continuity at the interface between regions for the thermal group: $J_2^1(a/2) = J_2^2(a/2)$;

iii) Flux continuity at the interface between regions for the thermal group: $\phi_2^1(a/2) = \phi_2^2(a/2)$;

iv) Null flux in the right boundary for the thermal group: $\phi_2^2(a/2+b) = 0$;

v) Even function for the thermal group: $\phi_2^1(-a/2) = \phi_2^1(+a/2)$;

vi) Power of slab reactor: $\int_{-a/2}^{+a/2} \sum_{g'=1}^{2} w\Sigma_{fg'}^1 \phi_{g'}^1(x)\,\mathrm{dx} + 2\int_{a/2}^{a/2+b} \sum_{g'=1}^{2} w\Sigma_{fg'}^2 \phi_{g'}^2(x)\,\mathrm{dx} = \mathrm{P}_o$;

vii) Flux continuity at the interface between regions for the fast group: $\phi_1^1(a/2) = \phi_1^2(a/2)$;

viii) Null flux in the right boundary for the fast group: $\phi_1^2(a/2+b) = 0$;

Fig. 1 shows the regions and slab reactor dimensions used in calculations and in Table 1 we have nuclear parameters for each fuel region and energy group. In the NEM [6], we defined the node 1 cm in size, so for each iteration the neutron diffusion equation is solved 240 times, while using the analytical solution, we solved only twice. To determine the number of times that the neutron diffusion equation was solved, we multiply the total number of nodes by the number of iterations. These data are shown in Table 2.

Figure 1: *Slab reactor with two fuel regions*.

Table 1: Nuclear parameters of a heterogeneous slab reactor with only fuels.

Region	g	D_g(cm)	$\Sigma_{rg}(\mathrm{cm}^{-1})$	$\nu\Sigma_{fg}(\mathrm{cm}^{-1})$	$\omega\Sigma_{fg}(\mathrm{cm}^{-1})$	$\Sigma_{gg'}(\mathrm{cm}^{-1})$
1	1	1.000	0.020	0.005	0.005	0.000
	2	0.500	0.080	0.099	0.099	0.010
2	1	1.500	0.026	0.010	0.010	0.000
	2	0.500	0.180	0.200	0.200	0.015

Table 2: Comparison of results for slab reactor with only fuels.

Method	Iterations	k_{eff}	Relative Error (%)	Number of Calculations
NEM	5741	0.9015965031	-	1377840
Analytical	40	0.9015965030	$1.109\text{x}10^{-8}$	80

The convergence parameters used were of $\varepsilon_k = 10^{-8}$ for the eigenvalue and $\varepsilon_\phi = 10^{-7}$ for the neutron flux. The power obtained in the reactor, using the NEM, was P_o = 30.149387. Fig. 2 shows the neutron flux distributions analytical - $\phi_g^n(\text{x})$ and numerical - $\bar{\phi}_g$ for two energy groups.

In these calculations, the average neutron flux for the two regions as well as the fission neutron source used in the power method are defined, respectively, as

$$\bar{\phi}_g^1 = \frac{1}{a}\int_{-a/2}^{+a/2} \phi_g^1(x)\,\text{dx}, \tag{21}$$

and

$$\bar{\phi}_g^2 = \frac{1}{b}\int_{a/2}^{a/2+b} \phi_g^2(x)\,\text{dx}, \tag{22}$$

and

$$s_f = \sum_{g'=1}^{2} \nu\Sigma_{fg'}^1 \bar{\phi}_{g'}^1 a + 2\sum_{g'=1}^{2} \nu\Sigma_{fg'}^2 \bar{\phi}_{g'}^2 b, \tag{23}$$

where the superscripts 1 and 2 denote the fuel regions.

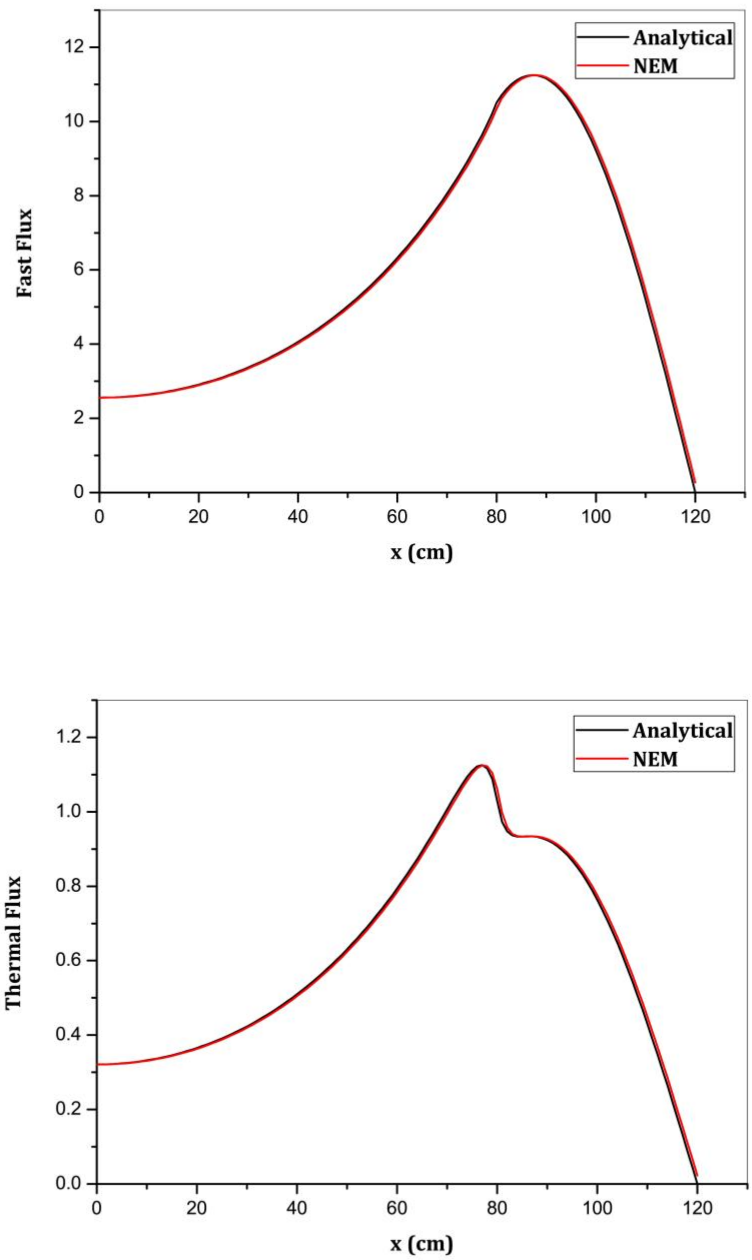


Figure 2: *Comparison of the neutron flux for fuel regions*.

Fig. 3 shows the flow chart used in the calculation of eigenvalue and neutron flux from the analytical solution.

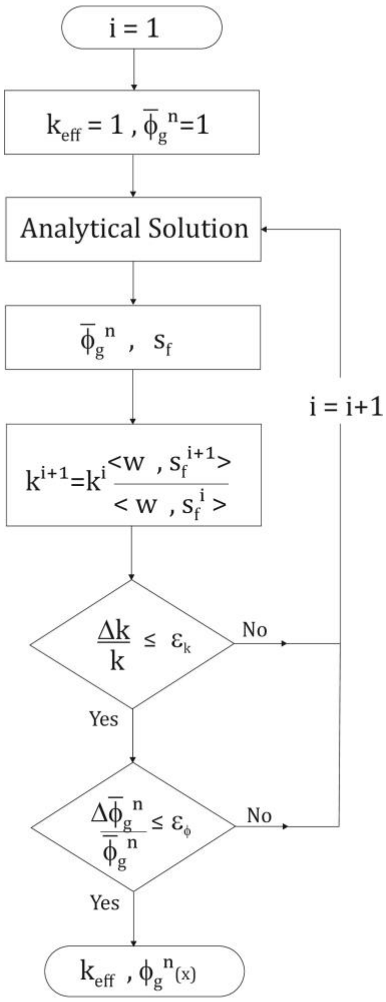


Figure 3: *Flow chart used in the analytical solution for the calculation of neutron flux.*

3.2. Fuel and reflector regions

For this case, we use the solution of the neutron diffusion equation for the fuel region, given by Eqs.(15) and (16) and the solution for the neutron flux for the reflector region, given by Eqs.(19) and (20). Table 3 shows the nuclear parameters used in these calculations. The power obtained in the reactor, using the NEM, was P_o = 6.87267085. The size of the regions of fuel and reflector are respectively, *a = 60 cm* and *b = 20 cm* as shown in Fig. 4. In this case, the boundary and continuity conditions are:

i) Null net current in the origin for the fast group: $J_1^1(0) = 0$;

ii) Current continuity at the interface between regions for the fast group: $J_1^1(a/2) = J_1^2(a/2)$;

iii) Flux continuity at the interface between regions for the fast group: $\phi_1^1(a/2) = \psi_1^2(a/2)$;

iv) Null flux in the right boundary for the fast group: $\psi_1^2(a/2 + b) = 0$;

v) Even function for the fast group: $\phi_1^1(-a/2) = \phi_1^1(+a/2)$;

vi) Power of slab reactor: $\int_{-a/2}^{+a/2} \sum_{g'=1}^{2} w\Sigma_{fg'}^1 \phi_{g'}^1(x)\,\mathrm{dx} = \mathrm{P}_o$;

vii) Flux continuity at the interface between regions for the thermal group: $\phi_2^1(a/2) = \psi_2^2(a/2)$;

viii) Null flux in the right boundary for the thermal group: $\psi_2^2(a/2 + b) = 0$;

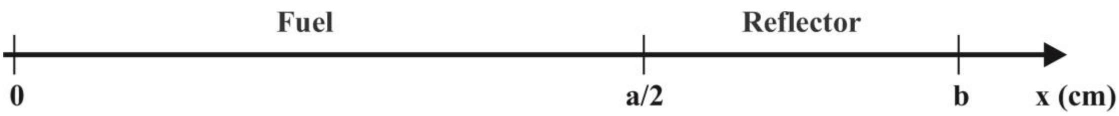


Figure 4: *Slab reactor with regions of fuel and reflector*.

Table 3: Nuclear parameters of a heterogeneous slab reactor with fuel and reflector.

Region	g	D_g (cm)	Σ_{rg} (cm^{-1})	$\nu\Sigma_{fg}$ (cm^{-1})	$\omega\Sigma_{fg}$ (cm^{-1})	$\Sigma_{gg'}$ (cm^{-1})
1	1	1.438000	0.029350	0.000242	0.000242	0.000000
	2	0.397600	0.104900	0.155618	0.155618	0.015630
2	1	1.871420	0.035411	0.000000	0. 000000	0.000000
	2	0.283409	0.031579	0.000000	0.000000	0.034340

Table 4: Comparison of results for slab reactor with fuel and refletor.

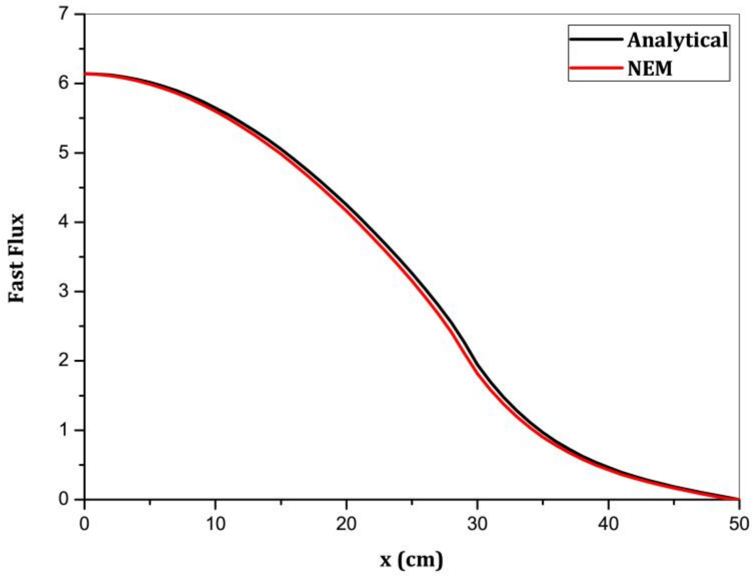
Method	Iterations	k_{eff}	Relative Error (%)	Number of Calculations
NEM	316	0.73491924915	-	31600
Analytical	33	0.7349192493	$1.360\text{x}10^{-8}$	66

The convergence parameters are the same used previously. The results are shown in Table 4. Fig. 5 shows the neutron flux distributions analytical - $\phi_g(\mathrm{x})$ and numerical - $\bar{\phi}_g$ for two energy groups. The average neutron flux and fission neutron source for fuel region used in the power method are:

$$\bar{\phi}_g^1 = \frac{1}{a}\int_{-a/2}^{+a/2} \phi_g^1(x)\,\mathrm{dx}, \tag{24}$$

and

$$s_f = \sum_{g'=1}^{2} \nu\Sigma_{fg'}^1 \bar{\phi}_{g'}^1 a, \tag{25}$$



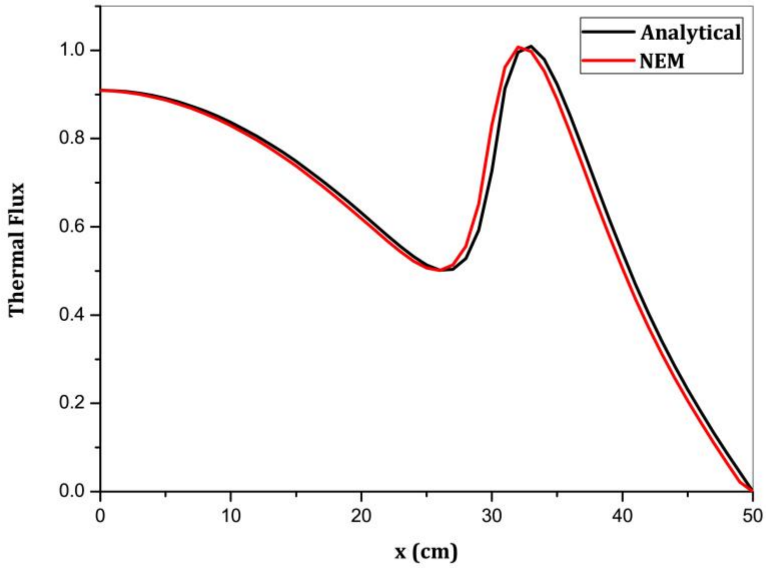


Figure 5: *Comparison of neutron flux for fuel and reflector regions*.

The results in both cases were quite satisfactory. For the analytical solution, the graphics were generated using the $\phi_g^n(\mathrm{x})$, while the NEM we used the average flux $\bar{\phi}_g^n$ at each node.

4. CONCLUSION

In this paper an analytical solution of the neutron diffusion equation was coupled with an iterative method to determine the neutron flux and eigenvalue in the reactor. The results obtained were compared to those from the numerical methods. The iterative method used in the calculation of eigenvalue was the power method. From the analytical solution, we calculate the average neutron fluxes and fission neutron sources, in each region, to be used in iterative process to determine the eigenvalue.

The results obtained by analytical solution were very accurate both in the calculation of neutron flux as well as in the calculation of eigenvalue. In both cases, we only use the reactor power as previously known information.

The greatest advantage of using analytical solutions is that these solutions are not depend of the region size, since the nuclear parameters in these regions are uniform. The same can't be observed when using numerical methods, especially the finite difference method.

This methodology can be extended to two or three dimensions, imposing flux and current continuity.

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