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Three-Dimensional Simulation of Neutron Flux Distribution in Boron Neutron Capture Therapy (BNCT)

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Abstract. Glioblastoma Multiforme (GBM) is one of the most aggressive and difficult-to-treat forms of malignant brain tumor, presenting a high incidence and resistance to conventional treatment methods. Boron Neutron Capture Therapy (BNCT) stands out as an innovative and promising approach for treating complex tumors such as GBM, as it enables the selective destruction of tumor cells with minimal impact on healthy tissues. In this study, the multigroup neutron diffusion equation is solved in a three-dimensional domain using four energy groups. The neutron source is represented as a boundary condition, and after diagonalizing the system of equations, the method of Separation of Variables can be applied to obtain an exact solution. The validation of the proposed approach was carried out through numerical simulations in a water phantom, whose results indicated that thermal and epithermal neutron fluxes are predominant.

Keywords. BNCT, Neutron Flux, Neutron Diffusion Equation, Exact Solution, Method of Separation of Variables

1 Introduction

Glioblastoma multiforme (GBM) is the most common and aggressive type of brain tumor. Classified as a glioma, it originates from glial cells, which provide support and protection to neurons. GBM is characterized by rapid and invasive growth, making complete removal difficult and leading to a high recurrence rate. Despite advances in medicine and cancer therapies, the prognosis for patients diagnosed with GBM remains challenging, with a survival rate of only 5% five years after diagnosis.

The choice of treatment for GBM is individualized, considering the tumor's location and extent, as well as the patient's response. Surgical resection is often chosen to remove as much tumor tissue as possible without compromising essential neurological functions. However, due to the infiltrative nature of GBM, complete removal is rarely achieved, making the use of additional therapies necessary. Radiotherapy and chemotherapy are widely employed to slow tumor progression. Furthermore, emerging approaches such as immunotherapy [1, 9] and Boron Neutron Capture Therapy (BNCT) [3–8, 13, 14] are being studied to enhance treatment efficacy and minimize damage to healthy tissues.

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BNCT utilizes the nuclear reaction between a neutron and the boron-10 isotope (^{10}B). This method is based on the administration of a compound containing ^{10}B, which selectively accumulates in tumor tissue. After this concentration, the patient is irradiated with neutrons, triggering a nuclear reaction that releases alpha particles and lithium-7 (^7Li) nuclei, both with high linear energy transfer. The boron capture reaction is described as follows:

$$n + {}^{10}B \rightarrow [{}^{11}B]^* \begin{cases} \longrightarrow {}^7Li + \alpha + 2.79 \text{ MeV } (6\%) \\ \longrightarrow {}^7Li^* + \alpha + 2.31 \text{ MeV } (94\%) \\ \qquad\qquad \downarrow \\ \qquad\qquad {}^7Li + \gamma \text{ (0.48 MeV)} \end{cases}$$

Figure 1: Boron capture reaction. Source: the authors.

The main advantage of BNCT lies in its high specificity for cellular damage, as the emitted particles have a short range—approximately 9 micrometers for alpha particles and 5 micrometers for lithium nuclei, totaling only 14 micrometers [10]. This range is smaller than the average cell diameter, ensuring that destruction occurs predominantly in tumor cells that have absorbed boron, while adjacent healthy cells are spared. Therefore, the precise determination of neutron and gamma dose rates is essential to ensure the safety and effectiveness of the treatment. Thus, BNCT represents a promising alternative for the treatment of tumors resistant to conventional therapies.

Historically, BNCT (Boron Neutron Capture Therapy) used nuclear reactors as a neutron source, as only these facilities could generate sufficiently intense thermal and epithermal neutron fluxes. Currently, there is a movement to replace reactors with accelerator-based neutron sources, which can be installed in hospitals, facilitating the spread of BNCT as a viable alternative in oncological treatment. Although few reactor-based facilities remain active (in Argentina, China, Japan, and Taiwan), these facilities continue to play a key role in advancing BNCT [2]. In Japan, since 2020, BNCT has been employed in the clinical treatment of inoperable head and neck carcinomas, using accelerator-based neutron sources. With the increasing number of patients undergoing this therapy, it has become essential to improve treatment planning systems to optimize the dose and maximize therapeutic efficacy [13].

Currently, Monte Carlo algorithms are the most commonly used methods for BNCT planning [3–5, 8, 13, 14], but there is a growing demand for faster and equally accurate methods for dose calculation. Studies have explored new approaches to improve the efficiency of dose calculations in BNCT. For example, [14] calculated neutron flux distributions in a head and neck phantom using multigroup diffusion equations, reducing computation time compared to the Monte Carlo method, but with lower accuracy. [7] proposes a hybrid method for calculating neutron flux in BNCT, combining Monte Carlo simulations with diffusion equations using DIF3D (finite difference method).

In this work, we aim to solve the multigroup neutron diffusion equation in a three-dimensional domain, considering four energy groups, with the goal of analyzing the behavior of the neutron flux used in BNCT treatment. To achieve this, the neutron source is placed at the boundary at $x = 0$, transforming the problem into a homogeneous formulation. Furthermore, the system of equations is diagonalized, allowing the decoupling of the differential equations and their independent solution. The final solution is obtained using the method of Separation of Variables. Unlike the works presented in the literature, the proposal of this study is to present a solution with lower computational time than the Monte Carlo Method and without the inherent approximations of numerical methods. Numerical simulations are presented on a water phantom, and the results obtained are consistent with those reported in the literature.

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2 Methodology

To model the neutron flux exiting a reactor or accelerator used in BNCT treatment, a phantom (a structure designed to simulate the physical and radiological properties of biological tissues) composed of water is considered to study the neutron distribution.

In Figure 2, a representative schematic of a cross-sectional view can be observed, where an orange structure represents the collimator of the irradiation system. The neutron beam (horizontal blue arrows) exits the collimator and enters the region of interest. These neutrons are directed to enter perpendicularly on the water phantom. Inside the phantom, there is a black dashed rectangle, indicating a region of interest where the neutron flux distribution will be analyzed.

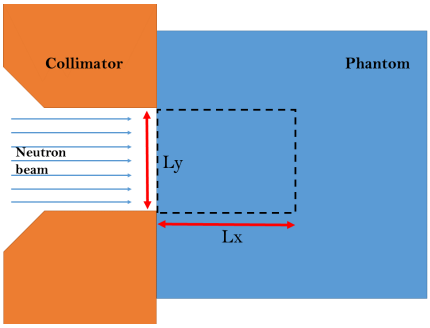

Figure 2: Cross-sectional view of the water phantom. Source: the authors.

To model this process, the following equation is a form of the stationary multigroup diffusion equation for neutrons, used to describe the distribution of neutron flux considering their interactions with the medium [11, 12]:

$$-D_g\nabla^2\Phi_g + \Sigma_{R,g}\Phi_g = \sum_{g'=1}^{g-1}\Sigma_{s,g'\to g}\Phi_{g'} + S_g, \tag{1}$$

where Φ_g is the neutron flux in group g, D_g is the diffusion coefficient, $\Sigma_{R,g}$ is the macroscopic removal cross section, $\Sigma_{s,g'\to g}$ is the macroscopic scattering cross section, and S_g is an external neutron source.

The approach proposed in this work consists of reformulating the neutron diffusion equation by treating the source as a boundary condition at $x = 0$. This strategy allows the application of the method of Separation of Variables, simplifying the analytical solution of the problem.

$$-D_g\nabla^2\Phi_g + \Sigma_{R,g}\Phi_g = \sum_{g'=1}^{g-1}\Sigma_{s,g'\to g}\Phi_{g'}. \tag{2}$$

When applying this formulation to a domain representing a region of brain tissue with a well-defined geometry, it becomes reasonable to assume homogeneous boundary conditions. These conditions impose that the neutron flux is zero at the start and end of each boundary of the domain, ensuring that no particles escape outside the considered region, except for the boundary at $x = 0$, where the neutron source $\Phi_g(0, y, z) = f$ will be applied. In this formulation, the function f is obtained by substituting $x = 0$ into the original source term, ensuring consistency between the modeling and the expected physical behavior.

For the application of the methodology, the Equation (2) is first rewritten in matrix form:

$$-\mathbf{D}\nabla^2\mathbf{\Phi} + \mathbf{\Sigma}\mathbf{\Phi} = \overline{0}, \tag{3}$$

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where $\mathbf{D}$ represents the diagonal matrix of diffusion coefficients, $\nabla^2\mathbf{\Phi}$ denotes the application of the Laplacian operator to the neutron flux vector $\mathbf{\Phi}$, $\mathbf{\Sigma}$ is the removal and scattering matrix between energy groups, and $\overline{0}$ is a null vector.

To decouple the system of equations and solve them independently, $\mathbf{\Sigma}$ is diagonalized. For this, a matrix $\mathbf{P}$ is used such that $\mathbf{P}^{-1}\mathbf{\Sigma}\mathbf{P} = \mathbf{\Lambda}$, where $\mathbf{\Lambda}$ is a diagonal matrix whose elements are the eigenvalues λ_i of the matrix $\mathbf{\Sigma}$, and $\mathbf{P}$ is composed of the eigenvectors of $\mathbf{\Sigma}$. Thus, a new unknown vector is defined as $\mathbf{\Psi} = \mathbf{P}^{-1}\mathbf{\Phi}$, and $\mathbf{\Phi} = \mathbf{P}\mathbf{\Psi}$ is substituted into Equation (3), yielding:

$$-\mathbf{D}\nabla^2\mathbf{\Psi} + \mathbf{\Lambda}\mathbf{\Psi} = \overline{0}. \tag{4}$$

Now, the decoupled partial differential equations can be solved for each energy group by applying the method of Separation of Variables: $\Psi_g(x, y, z) = X(x)Y(y)Z(z)$. Substituting this expression into the original PDE for each group and considering $\gamma_g = \frac{\lambda_i}{D_g}$, a set of ordinary differential equations is obtained, whose solutions are well known. Thus, the solution for Ψ_g is:

$$\Psi_g = \sum_{m=1}^{\infty}\sum_{l=1}^{\infty} A_{l,m}\left[-e^{-2\xi_{3,l,m}L_x}e^{\xi_{3,l,m}x} + e^{-\xi_{3,l,m}x}\right]\sin(\xi_{2,m}y)\sin(\xi_{1,l}z), \tag{5}$$

where $\xi_{1,l} = \frac{l\pi}{L_z}$, with $l = 1, 2, \ldots$; $\xi_{2,m} = \frac{m\pi}{L_y}$, with $m = 1, 2, \ldots$; and $\xi_{3,l,m} = \sqrt{\gamma_g + \xi_{2,m}^2 + \xi_{1,l}^2}$. The non-homogeneous boundary condition is used to determine the constants $A_{l,m}$. Finally, it is sufficient to revert to the original variable $\mathbf{\Phi} = \mathbf{P}\mathbf{\Psi}$ to obtain the final solution of the problem.

2.1 Results and Discussions

The numerical simulation of the solution found to determine the behavior of the neutron flux was performed in Python. Four energy groups were used, where Group 1 covers energies between 1.0×10^3 and 3.0×10^5 eV, Group 2 includes neutrons with energies ranging from 10 to 1.0×10^3 eV, Group 3 encompasses neutrons with energies between 0.4 and 10 eV, while Group 4 has an energy range from 0 to 0.4 eV. For the energy group intensities related to the non-homogeneous boundary condition, an approximation was used where a function is inversely proportional to the mean energy range of each group [11, 12]. The values of the diffusion coefficients and cross-sections are presented in Table 1. The domain considered for the simulation has dimensions $L_x = 5.0$, $L_y = 3.0$, and $L_z = 3.0$, with grid spacings $\Delta x = 0.1$, $\Delta y = 0.1$, and $\Delta z = 0.1$, using $L = M = 20$ terms.

Table 1: Parameters used in the numerical simulation. Source: Adapted from [11, 12].

g	D_g [cm]	$\Sigma_{R,g}$ [1/cm]	$\Sigma_{s,g'-g}$ [1/cm] (g-1→g)	$\Sigma_{s,g'-g}$ [1/cm] (g-2→g)
1	2.0×10^{-1}	1.572×10^{-1}	-	-
2	2.5×10^{-1}	1.1×10^{-1}	6×10^{-2}	-
3	2.2×10^{-1}	9.7×10^{-2}	6.1×10^{-2}	-
4	2.1×10^{-2}	2.2×10^{-3}	0	5.228×10^{-2}

Figure 3 illustrates the distribution of fluxes as a function of depth x in the phantom, at the center of the mesh of y and z. It can be observed that the neutron fluxes decrease exponentially as the depth increases. It is also noted that the thermal and epithermal fluxes are more significant, which is in line with expectations for BNCT therapy, while the high-energy fluxes are nearly insignificant (close to zero).

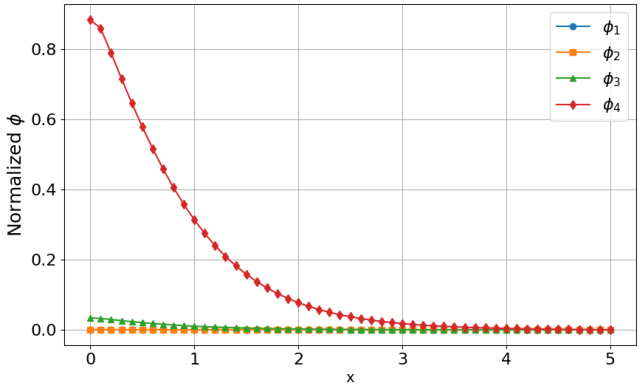
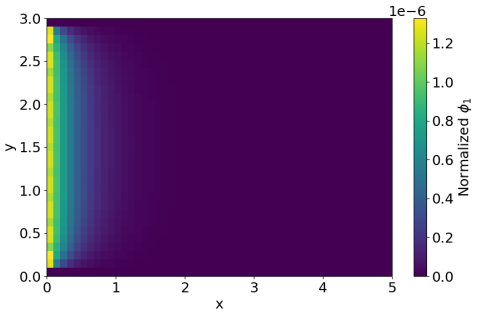
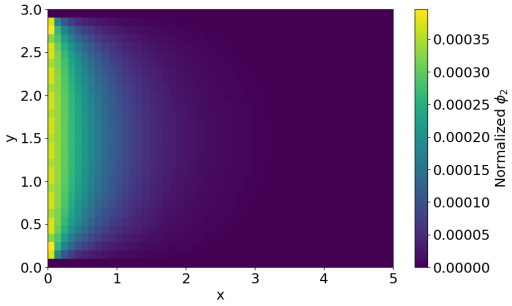


Figure 3: Flux distribution as a function of depth x in the phantom, in the middle of the y and z grid. Source: the authors.

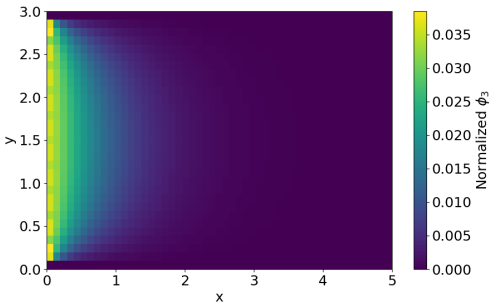
The Figure 4 shows the heatmaps of ϕ_1, ϕ_2, ϕ_3, and ϕ_4, respectively, in the plane at the midpoint of the mesh in the z-direction. It can be observed that the fluxes ϕ_1 and ϕ_2 tend to zero at the initial positions. The fluxes ϕ_3 and ϕ_4 decrease more gradually, as they lose energy progressively while interacting with the atoms of the medium (moderation effect).



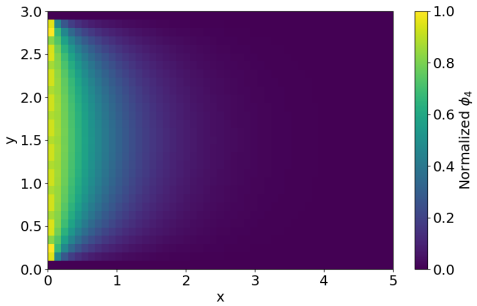
(a) Heatmap of ϕ_1.



(b) Heatmap of ϕ_2.



(c) Heatmap of ϕ_3.



(d) Heatmap of ϕ_4.

Figure 4: Heat maps of the variables ϕ_1, ϕ_2, ϕ_3, and ϕ_4 in the plane at the midpoint of the mesh in the z-direction. Source: the authors.

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3 Final Considerations

In this work, the solution to the multigroup neutron diffusion equation in a three-dimensional domain was presented, considering four energy groups. The behavior of the neutron flux employed in BNCT therapy for the treatment of GBM was studied. The approach used treats the neutron source, characteristic of the BNCT treatment, as a boundary condition at $x = 0$, homogenizing the problem and allowing the application of the method of Separation of Variables. Moreover, the system of equations was diagonalized, enabling the decoupling of the differential equations and their solution independently. It is worth noting that this study allows obtaining an analytical solution, i.e., without the truncation errors inherent in numerical methods, and with reduced computational effort. Although the solution is analytical, it is expressed as an infinite series which, in practice, must be truncated to a finite number of terms. This truncation introduces a small approximation error, and the computational effort required depends on the number of terms considered in the series. The simulated results are in accordance with the dynamics of the problem.

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