



# Maxwell Spectrum as a Parameter to Verify the Dose in Brain Cancer (Glioblastoma) by Boron Neutron Capture Therapy (BNCT) using Monte Carlo Method

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**Abstract:** To evaluate the efficiency of neutron capture therapy (BNCT) treatment in glioblastoma multiforme, it is necessary to evaluate the impact of the neutron beam on the tumor cell and find better results so that BNCT treatment is viable. Glioblastoma multiforme is one of the most lethal cancers and conventional radiotherapy is almost ineffective for this type of tumor. Among several approaches to describe the procedure and the neutron spectrum, the Maxwell spectrum in the epithermal neutron range was used. For this,  $T=0.0025$  MeV was used to describe this spectrum. MCNP software was used to simulate a BNCT treatment using the Maxwell spectrum to describe the neutron source. The user provided the quantities of interest, such as fluence and dose. These are extremely important quantities to describe a BNCT planning protocol. A concentration of 30 ppm of Boron-10 was simulated in the tumor. Output data provides normalized values. It was necessary to carry out some mathematical operations to obtain values closer to reality. Thus, a dose of 32 Gy was obtained for the Maxwell spectrum described with  $T=0.0025$  MeV and a neutron fluence of  $1.5 \times 10^{12}$  n/cm<sup>2</sup>. The values calculated based on the simulation in MCNP5 described by an epithermal neutron source obeying a Maxwellian function, were in agreement with the reference values in the literature.

**Keywords:** BNCT, Maxwell, MCNP, Dose, Neutron.



# Espectro de Maxwell como Parâmetro para Verificar a Dose em Câncer Cerebral (Glioblastoma) por Terapia por Captura de Nêutrons pelo Boro (BNCT) Utilizando o Método de Monte Carlo

**Resumo:** Para avaliar a eficiência do tratamento com terapia por captura de nêutron (BNCT) em glioblastoma multiforme, é necessário avaliar o impacto do feixe de nêutron na célula tumoral e encontrar melhores resultados para que o tratamento com BNCT seja viável. O glioblastoma multiforme é um dos tumores mais letais e a radioterapia convencional é quase ineficaz para este tipo de tumor. Entre várias abordagens para descrever o procedimento e o espectro de nêutrons, foi utilizado o espectro de Maxwell na região de nêutrons epitérmicos. Para isso, foi utilizado  $T=0,0025$  MeV para descrever este espectro. O software MCNP foi utilizado para simular um tratamento BNCT utilizando o espectro de Maxwell para descrever a fonte de nêutrons. O usuário forneceu as quantidades de interesse, tais como a fluência e a dose. Estas são quantidades extremamente importantes para descrever um protocolo de planejamento BNCT. Uma concentração de 30 ppm de Boro-10 foi simulada no tumor. Os dados de saída fornecem valores normalizados. Foi necessário efetuar algumas operações matemáticas para obter valores mais próximos da realidade. Assim, obteve-se uma dose de 32 Gy para o espectro de Maxwell descrito com  $T=0,0025$  MeV e uma fluência de nêutrons de  $1,5 \times 10^{12}$  n/cm<sup>2</sup>. Os valores calculados com base na simulação em MCNP5 descrita por uma fonte de nêutrons epitérmica obedecendo a uma função Maxwelliana, estavam de acordo com os valores de referência da literatura.

**Palavras-chave:** BNCT, Maxwell, MCNP, Dose, Nêutron.

## 1. INTRODUCTION

Neutron Capture Therapy, better known by its acronym BNCT (Boron neutron Capture Therapy) is a binary technique that consists of first introducing a boron compound into the patient and then irradiating them with a neutron beam. The idea of using neutrons to treat tumors arose in 1936, shortly after the discovery of the neutron in 1932. Studies since then have shown great efficiency in combating brain cancer (Glioblastoma) [1], and are not limited to this type of tumor. Glioblastoma multiforme (GBM) is one of the cancers whose survival can be increased with the use of BNCT. This type of tumor is characterized by "tentacles" that grow very quickly and spread throughout the brain. These tumors are often inoperable and, when treated with conventional radiotherapy, affect patients mental capacity. BNCT has therefore emerged as a way of treating this type of tumor, given the ineffectiveness of chemotherapy, conventional radiotherapy and surgery.

In conventional radiotherapy, a linear accelerator is used to produce photons and/or electrons. In BNCT, the most researched form of treatment is in a research nuclear reactor, which produces epithermal neutron beams of approximately  $10^{-6}$  MeV to  $10^{-2}$  MeV (where eV is a unit of energy named electron volt) with a fluence of  $10^{12}$  n/cm<sup>2</sup>. There are currently linear neutron accelerators with the function of BNCT treatment.

The idea behind BNCT treatment is to minimize the effects of radiation on healthy cells and maximize the same effects on tumor cells. This is done by applying a boron compound, containing boron-10, which is a stable isotope. The prescription for this chemical compound is a non-toxic, non-radioactive isotope with an isotopic abundance of 20%. Currently, borophenylalanine (BPA) and sodium mercaptoundecahydro-closododecaborane ( $\text{Na}_2\text{B}_{12}\text{H}_{11}\text{SH}$ ) are the most widely used compounds for BNCT. These

compounds have made selectivity in the tumor acceptable, in which the healthy tissue-tumor ratio is 1:4.

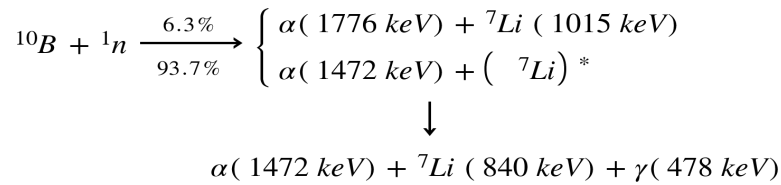
$^{10}\text{B}$  has a shock section of 3843 barns [5] for epithermal neutrons. The consequence of this is the neutron's high interaction power with  $^{10}\text{B}$ . Among the different interactions of the neutron with the material, neutron capture stands out. Neutron capture by boron produces a nuclear reaction of the form  $^{10}\text{B}(n;\alpha)^7\text{Li}$ . In this reaction, the neutron is absorbed by the boron and the product of this reaction is the release of an alpha particle and a Lithium-7 ( $^7\text{Li}$ ) atom. The diagram is shown in figure 1.

In the neutron capture process,  $^{10}\text{B}$  transmutes into  $^{11}\text{B}$  which is highly unstable and almost instantaneously decays into metastable or stable  $^7\text{Li}$ , in which the former releases gamma radiation with an energy of 478 keV, which is largely responsible for energy deposition in regions outside the tumor. Both the alpha particle and  $^7\text{Li}$  have high linear energy transfer (LET), i.e. they transfer a lot of energy per unit path. The high LET means that the products of nuclear reactions in the tumor (except gamma rays) deposit all, or at least almost all, of their energy locally.

The alpha particle and  $^7\text{Li}$  have a LET of 164 keV/ $\mu\text{m}$  and 151 keV/ $\mu\text{m}$  respectively, with a tissue range of 9  $\mu\text{m}$  and 5  $\mu\text{m}$ .

The deposition of high energy in the tumor, and consequently a high dose, causes the DNA damage necessary for tumor cell apoptosis. The tissues adjacent to the tumor are hardly affected, since almost all the energy has been deposited in the tumor. In addition to the dose caused by the  $^{10}\text{B}(n;\alpha)^7\text{Li}$  reaction, in 94% of the reactions gamma rays of 0.48 MeV energy are also released. However, this contribution is practically negligible, as it causes little biological effect [6,7]. Figure 1 shows the nuclear reaction that takes place inside the cell with boron and the respective energies released.

**Figure 1:** Neutron capture reaction by boron



In order to be able to verify the necessary physical quantities, such as neutron fluence, dose, among others, it is necessary to use methods that can measure and statistically provide the results. Computer simulation using the Monte Carlo method was used to generate the results. The MCNP5 software was used to carry out the simulation and generate the output data, once programmed. The VISED program was used to provide an image as a visualization facilitator, making the program more aesthetic, since there is an associated geometry.

## 2. MATERIALS AND METHODS

### 2.1. Monte Carlo Method

The Monte Carlo method is a computational method that uses random numbers and statistics to solve problems. Simulating a probabilistic model consists of generating stochastic mechanisms and then observing the resulting flow of the model over time. A general framework built around the idea of "discrete events" has been developed to help follow a model over time and determine the relevant amount of interest.

In Brazil, it is currently impractical to carry out BNCT experiments on humans, as the method is still under development. In eastern countries, such as South Korea, BNCT treatments already exist in hospitals. A priori, the most appropriate way is to simulate the treatment using radiation and particle transport software. MCNP5 (Monte Carlo N-Particles) was the software used to simulate BNCT in this work. The software allows the user to

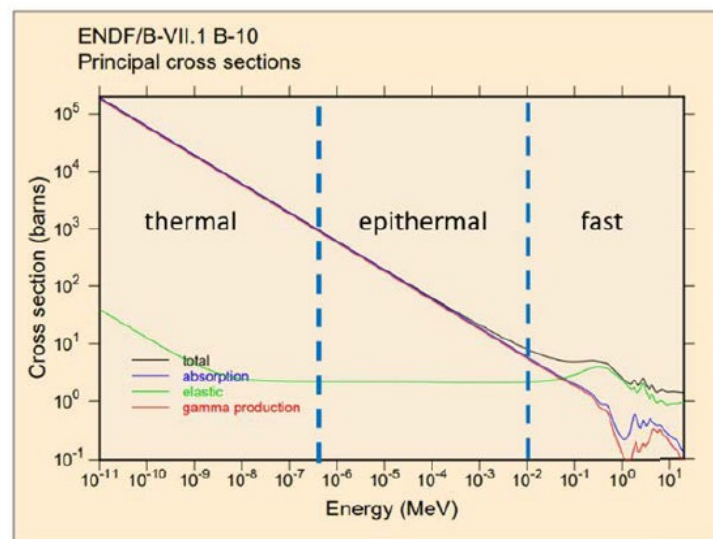
provide the input data and program the geometry of the system according to the syntax of the program language.

A head and neck phantom was used. VISED, a program that allows geometric visualization of the image generated by the code, was used to visualize the input data.

## 2.2. Neutron Spectrum

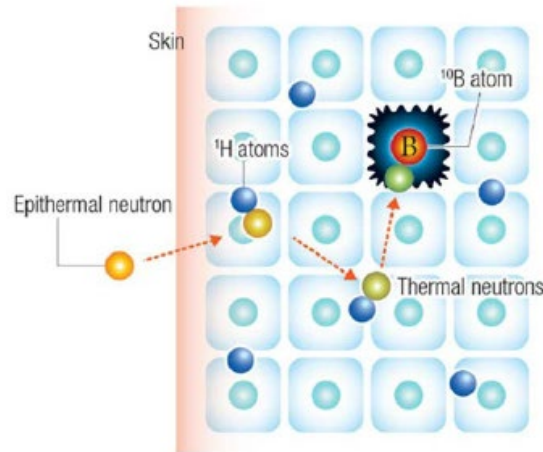
In BNCT treatment, a beam of neutrons is irradiated towards the region of interest. The impact of the neutron radiation damage on the material depends on the shock section and the energy of the neutron. For different energies, this impact can change. Boron has a high shock section for epithermal and thermal neutrons, as shown in figure 2.

**Figure 2:** Cross section in barns of  $^{10}\text{B}$  for neutrons as a function of energy. All interactions (total, absorption, elastic, gamma production) are shown.



The ideal neutron range for BNCT treatment is in the epithermal range (1 eV to 10 keV). This is because human tissue is rich in hydrogen, an element that acts as a good neutron moderator and the neutron loses part of its energy when it is moderated. The interest in using the BNCT technique lies in having the tumor hit by thermal neutrons. This is why epithermal neutrons are used as a source, as they are thermalized by the hydrogen in the tissue until they reach the tumor in the thermal range.

**Figure 3:** Neutron path being thermalized by the tissue. The hydrogen in the tissue is the main element for thermalizing the neutron.



Source: IAEA [11]

### 2.3. Characterization of the neutron source

The tumor is the object of study and so the irradiation field will be as small as possible to irradiate the region of interest. The source data in the MCNP software is shown in Table 1.

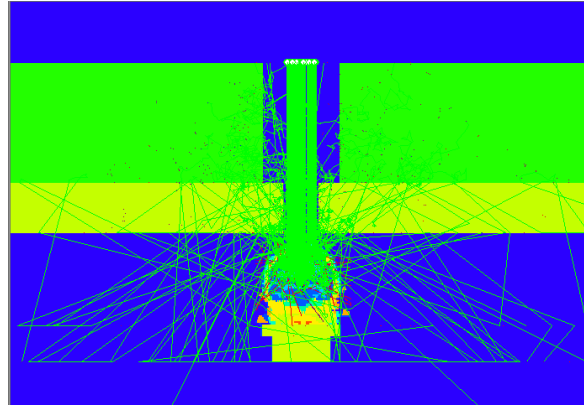
**Table 1:** Characteristics of the irradiation source

SOURCE GEOMETRY	CYLINDRICAL
Radius (cm)	3
Direction	-z
Particle	Neutron

The neutron source needs to be described by a neutron spectrum with a higher probability in the epithermal and thermal region. For this, the Maxwellian was used. The direction and direction of the neutron are shown in figure 4.



**Figure 4:** Image generated by VISED of Zubal phantom demonstrating the direction of the neutron beam source in the irradiation channel. The yellow region is the collimator (avoiding unnecessary irradiation).



In a gas, the energies of atoms and molecules are distributed according to the Maxwell-Boltzmann distribution function [8].

$$N(E) = \frac{2\pi N}{(\pi kT)^{3/2}} \cdot \sqrt{E} \cdot e^{-(E/kT)} \quad (1)$$

Simply put,

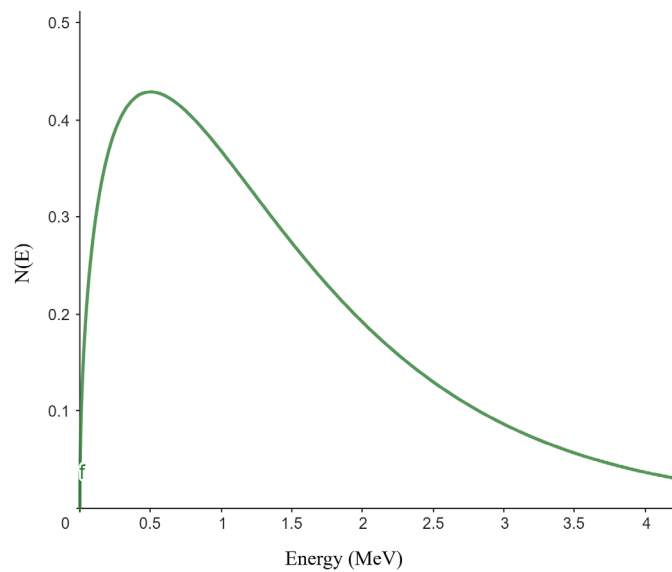
$$N(E) = CE^{1/2} \exp(-E/T) \quad (2)$$

Where,

- N(E) is the density of particles per unit volume, i.e. the density of particles;
- E the energy;
- T the absolute temperature of the medium or the characteristic energy of the process.

The Maxwell-Boltzmann equation was formulated empirically to describe the neutron energy in a fission spectrum, where T is an empirical adjustment parameter related to the nuclear temperature, i.e. the most probable energy of the spectrum. Figure 5 shows the Maxwellian function described by equation 2.

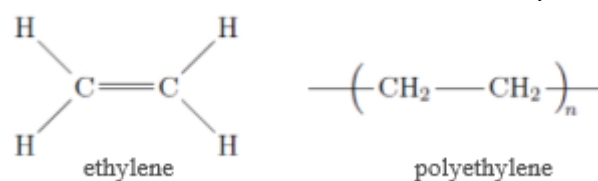


**Figure 5:** Maxwellian distribution function


The Maxwell spectrum described by equation 1 is configured so that the neutron density per energy  $N(E)$  is higher in the epithermal range, since the source was configured at a distance of a few cm from the scalp. This adjustment to the equation provides a good spectrum for BNCT treatment, for a temperature of 0.0025 MeV and figure 8 shows the spectrum obtained ( $T=0.0025$  in equation 2).

## 2.4. Collimator

A collimator was simulated to avoid irradiating uninteresting regions. The material used was polyethylene (PE), as it is a polymer with a high hydrogen content and does not favor secondary scattered radiation. Pure polyethylene is made up of carbon and hydrogen chains, as shown in figure 6.

**Figure 6:** Representations of the chemical structures of ethylene and polyethylene.


Source: Pereira [3]

In addition, carbon is an element that is stable to neutron reactions and has a low atomic mass (12.011 u). This makes it a good moderator for neutrons, which lose their kinetic energy by colliding inelastically and elastically with carbon and hydrogen atoms. The collimator is a planning tool and can be produced in different shapes and sizes depending on the location of the tumor. Whether or not it is used depends on the planning.

## 2.5. Planning

Several parameters are important in BNCT. The dose to the tumor and the neutron fluence used are essential parameters for the process to work properly. The patient is positioned in such a way that the neutron beam takes the shortest path to the tumor, as long as the surface of incidence is the scalp, which is the region located between the upper nuchal lines of the occipital bone and the supraorbital margins of the frontal bone. The tumor should not be irradiated by directly hitting the sinuses or neck, as the thermalization of the neutrons causes them to deposit energy in healthy tissues adjacent to the tumor and these regions are very sensitive to radiation (eyes and thyroid). This is why irradiation of these regions should be avoided.

For this simulation of Glioblastoma treatment, a distance between the scalp and the collimator of 3 cm was planned. The neutron beam is collimated in order to avoid secondary radiation reaching areas of no interest, i.e. healthy tissue. The distance between the scalp and the irradiation channel should also be avoided. If the distance is too great, part of the neutrons will be lost through the processes of radiation interaction with matter. In other words, the medium will absorb more neutrons than necessary, affecting the proper functioning of the procedure. The consequence of this is a decrease in the neutron flux and, consequently, the dose deposited in the tumor.

The minimum flux ( $\phi$ ) for BNCT treatment and the minimum dose in the tumor are, respectively,  $\phi = 10^9 \text{ cm}^{-2} \cdot \text{s}^{-1}$  and  $D = 20 \text{ Gy}$  [8,11,12]. However, it was used in this simulation  $= 10^{13} \text{ cm}^{-2} \cdot \text{s}^{-1}$ .

## 2.6. Dose Calculation

BNCT dose calculation differs from conventional radiotherapy. The BNCT dose takes into account radiation damage of different types. Some weight factors are integrated into the calculation, such as:

- Relative Biological Efficacy (RBE): Quantifies differences in biological efficacy for different qualities of radiation.
- Compound Biological Effectiveness (CBE): Radiobiological effect due to an exogenous compound.

The interaction of the neutron with the different elements of the human body produces particles and ions that deposit their energy locally or far away from the place where they were produced, in the case of gamma rays.

A standard model has been described for a dose calculation in which the dose per photon produces the same effect on a biological system as a dose delivered under the same conditions as a BNCT treatment. This model is called isoeffective dose and has a unit of Gy(W), Gy-RBE or Gy-Eq. The definition of dose does not change, but it is necessary to differentiate, since there are weight factors involved and the dose calculation delivered in BNCT cannot be converted directly into a dose calculation delivered by photon. Therefore, the dose delivered in a BNCT treatment can be converted into dose per photon using the isoeffective dose calculation, this calculation is given by equation 3.

$$D_{isoE} = w_1D_1 + w_2D_2 + w_3D_3 + w_4D_4 \quad (3)$$

Where,

$$D_1 = D_b, D_2 = D_N, D_3 = D_H, D_4 = D_\gamma$$

**Table 2:** The meaning of the components, their reactions and element of origin. For each dose component there is an energy and RBE associated.

SYMBOL	COMMON NAME	ORIGINATING REACTIONS
$D_b$	Boron dose	The $^{10}\text{B}(n,\alpha)^7\text{Li}$ reaction
$D_N$	Nitrogen dose	The $^{14}\text{N}(n,p)^{14}\text{C}$ reaction and 583 keV protons.
$D_H$	Hydrogen, fast neutron dose,	Energy is released by recoiling protons. Interaction with fast and epithermal neutrons
$D_\gamma$	Photon dose	Radiative capture within the patient mainly from the $^1\text{H}(n,\gamma)^2\text{H}$ reaction

The dose is mostly deposited by the  $^{10}\text{B}(n,\alpha)^{10}\text{Li}$  reaction. Of the four forms of energy deposition, 90% is caused by boron and the other 10% is distributed among the other reactions.

However, for this work we are not interested in calculating the isoeffective dose, but rather the gross dose delivered to the tumor. In BNCT, the dose is commonly calculated using the *kerma*, (an acronym for kinetic energy released per unit mass) approximation for neutrons and photons, applying the flux to *kerma* conversion factor. The flux to *kerma* conversion factor used was obtained by the International Commission on Radiation Units and Measurements (ICRU) 46 [9].

In the MCNP5 software, fluence was acquired as a quantity of interest.

### 3. RESULTS AND DISCUSSIONS

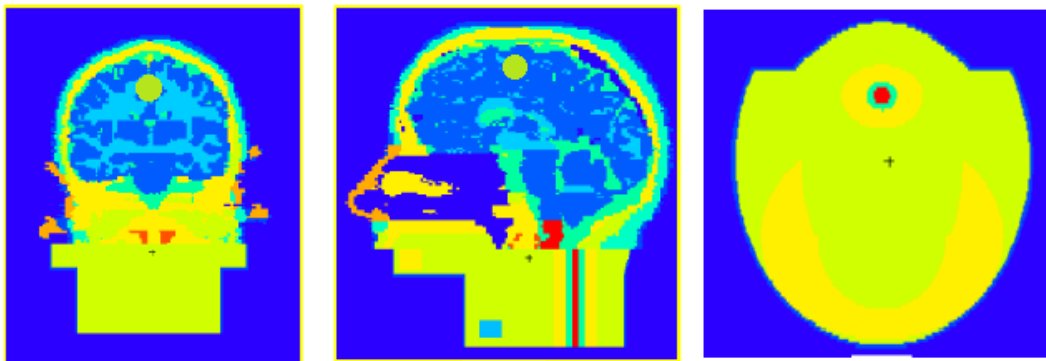
#### 3.1. Simulation with MCNP5

In MCNP, the user provides input data containing the materials and source, geometry and execution parameters. The output data then provides the values and quantities of interest.

A virtual head and neck phantom, programmed in MCNP, was used in this work, since the region of interest is the brain.

The phantom's code was modified. The modifications included the insertion of a tumor cell, with materials defined by ICRU 46, which was taken as a reference for describing the elements of the brain as well. The tumor, 2 cm in diameter and 4 cm from the scalp, was simulated in order to check the dose and flow in it. Table 1 shows the elements of the tumor's composition and figure 7 shows the image generated by VISED. The code that generates the image is the same that provides the output data. You can clearly see the divisions of the brain, head and sinuses. The small green circle at the top of the brain represents the tumor. These regions are the most affected by BNCT radiation, which is why the image and the qualitative description of the process are so important.

**Figure 7:** Zubal phantom (modified). Left to right: xz plane, yz plane, xy plane.



**Table 3:** Elements used to define the tumor considering 30 ppm of boron, which, 30 ppm =  $1.3 \cdot 10^{23}$  atom density.

ELEMENT	ATOMIC DENSITY ( $10^{24}$ )	ATOMIC FRACTION (%)
H	6.40E-02	0.1
O	2.69E-02	0.659
C	6.02E-03	0.185
N	1.18E-03	0.042
Na	5.60E-04	0.014
B-10	1.30E+23	3.00E-05

In the MCNP5 software, a neutron beam was programmed like the one described in this work, describing a Maxwellian distribution function (figure 8). The flux was the quantity

of interest and what is called a Tally, a quantity of interest, was used. The user provides the tally in the region they want to obtain and the program returns the value. For example, if the user wants to check the dose in MeV/g in a certain region, they provide the F6 in that region and the software returns a numerical value related to F6 (dose). Table 4 shows the definitions of each Tally.

The user enters the tally in the input and MCNP5 gives us the values in the output.

**Tabela 4:** Tallies types.

TALLY	PHYSICAL QUANTITY	UNIT
F1	Total current through a surface	particles
F2	Average flow through a surface	particles/cm <sup>2</sup>
F4	Average flow in a cell (volume)	particles/cm <sup>2</sup>
F5	Flow in point detector	particles/cm <sup>2</sup>
F6	Total energy deposited in a cell	MeV/g
F7	Total fission energy deposited in a cell	MeV/g
F8	Energy pulses	Pulses

Source: MCNP6 manual [12].

Therefore, the F4 tally was entered so that the software could provide the numerical value of the flow in the output channel. The flow conversion factors in *kerma*, according to ICRU 46, were applied to the tumor cell in order to obtain the dose in it, since there is a flow value in the tumor cell as well, but only the dose value was prioritized, so the numerical value of the flow in the tumor was not highlighted at this point.

The tallies are applied to the cell card, in which each cell corresponds to a specific region. The tumor, for example, is a cell on which the F4 tally has been applied.

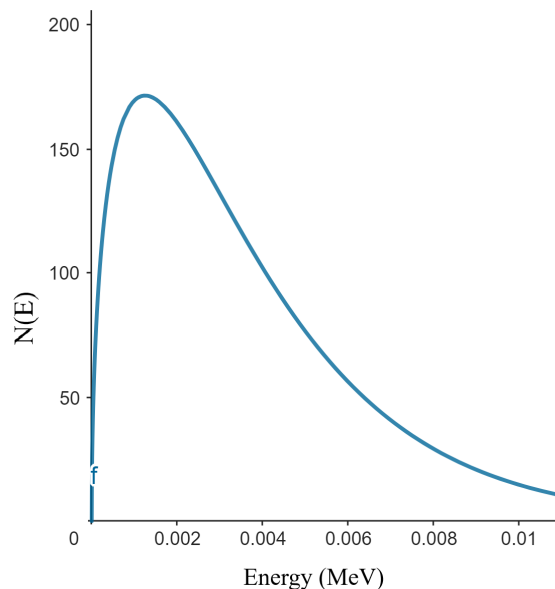
The accuracy of the values depends on the computational time and the number of tallies. The greater the number of stories, the longer the computational time and the more accurate the result. For this work, the code was written to run according to the number of

stories. To do this, 3 million stories were chosen, which required a computational time of 21.86 minutes.

### 3.2. Dose calculation

Equation 2 describes a Maxwellian distribution. Applying the condition where  $T=0.0025$  MeV shows a high density for neutrons in the epithermal range. This range is a good approximation for BNCT treatment, since neutrons lose energy when interacting with tissues and reach the tumor in the thermal range.

**Figure 8:** Maxwellian distribution function for  $T=0.0025$  MeV.



The dose in the tumor was obtained using the F4 tally (which provides the flow in the selected cell) and applying the flow-to-*kerma* conversion factors. These factors were placed in the input and the output provided the value of the total dose deposited per unit area, which is the unit of the conversion factors.

The value found in the output was,

$$D_N = 4.503 \cdot 10^{-13} \text{ cGy} \cdot \text{cm}^2 = 4.503 \cdot 10^{-15} \text{ cGy} \cdot \text{cm}^2 \quad (4)$$



This value is normalized, i.e. per particle, since the value provided by MCNP is given in that way.

To obtain an acceptable planning value for this treatment, we will use a value of 30 Gy-Eq [12] as a reference.

To obtain this equivalent dose value, is necessary a flux value of a flux of around:

$$\phi = 7 \cdot 10^{15} \frac{\text{neutrons}}{\text{cm}^2 \cdot \text{s}} \tag{5}$$

Then, multiply the flux given above, the value obtained was,

$$D_{real} = 4.503 \cdot 10^{-15} \cdot 7 \cdot 10^{15} \simeq 31.5 \text{ Gy} \tag{6}$$

The normalized dose was multiplied by the flux, because the flux provides the amount of neutrons in the cell, in other words, the original value of dose.

**Table 5:** Comparison between the supplied and calculated values with the reference values.

	MCNP	CALCULATED	REFERENCE
Volume (cm <sup>3</sup> )	4.18879	4.18879	—
Fluence (n . cm <sup>-2</sup> )	1.83627 · 10 <sup>-3</sup>	7 · 10 <sup>15</sup>	>10 <sup>9</sup>
Dose (Gy/cm <sup>2</sup> )	4.503 · 10 <sup>-15</sup>	31.5	20-50

## 4. CONCLUSIONS

In conventional radiotherapy, doses are administered fractionally, in which the patient receives a daily dose of 1.5 to 3 Gy over a period of 3-7 weeks [11]. In BNCT the dose is administered in a single fraction, in which the equivalent dose must be equal to the total administered by conventional radiotherapy.

Various uncertainty analyses have concluded that a reasonable uncertainty in the total dose distribution is 7.0%, excluding the uncertainty in the boron concentration in the tissues.

Therefore, taking an ideal dose of 30 Gy as a reference, the value that was calculated of a dose of 32 Gy is within the acceptable range for treatment. Not only the dose, but also the time, 21.86 minutes, which is an acceptable time for BNCT treatment.

The more precise the value, the more accurate the treatment. However, in order to achieve this accuracy, a greater number of histories need to be programmed into the MCNP, which would consequently lead to a longer treatment time. It is therefore necessary to work with the correct variables so that BNCT planning is feasible in terms of time, dose and flow.

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