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Investigation of the optimum neutron energy spectrum for brain tumor boron neutron capture therapy using Monte Carlo N-Particle Transport Code

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Abstract. Boron neutron capture therapy, a targeted technique for cancer treatment, is based on fission reaction of implanted boron-10 in tumor cells by thermal neutrons to yield alpha particles and recoiling lithium-7 nuclei. The short range of these ionizing fission products induces damage to the cancer cells while sparing surrounding healthy tissues. A methodology to determine the optimum neutron energy according to the depth of the tumor in the brain is developed in this work. This methodology mainly depends on separately considering the different reaction types at discrete neutron energies using Monte Carlo N-Particle Transport Code and investigating their relative contribution to the absorbed dose in both the tumor and surrounding healthy tissues. For a certain tumor depth, the neutron energy that maximizes the dose to the tumor and minimizes it in the surrounding healthy tissues is selected. The metrics to evaluate improvement in the optimization process are developed based on the ratio of the tumor dose rate density ($Gy/cm^3 \cdot s$) to that of the surrounding healthy tissues. The results showed a significant improvement when compared with those of the International Atomic Energy Agency recommended neutron energy ranges. For deep-seated tumors, the dose ratio was improved from 0.89 to 1.77 for tissues preceding the tumor and from 2.40 to 12.0 for tissues after the tumor. For the shallow-seated tumors, the dose ratio was improved from 2.48 to 2.64 for tissues preceding the tumor and from 8.63 to 18.8 for tissues after the tumor.

Keywords: Boron Neutron Capture Therapy, Brain Tumor, Neutron Radiotherapy, Dose, Monte Carlo N-Particle.

1. Introduction

Over the last few decades, radiation therapy has advanced to state-of-the-art modalities, which have considerably improved the survival rates among cancer patients. Amongst these, boron neutron capture therapy (BNCT) is a technique based on non-radioactive boron-10 (^{10}B) thermal neutron (~0.025 eV) capture to yield high linear energy transfer (LET) α-particles and recoiling ^{7}Li nuclei. The BNCT technique is highly selective because the ranges of these two particles (~8 μm and ~5 μm respectively) [1] are similar to those of typical cells. Consequently, radiation damage occurs mainly in the malignant cells while eluding the healthy surrounding cells, thus reducing the occurrence of radiation-induced secondary tumors [2].

The effectiveness of the BNCT treatment modality depends mainly on the selective delivery of ^{10}B to the tumor cells. The commonly used delivery agents are ^{10}B-4-borono-L-phenylalanine (10BPA) [3] and

sodium borocaptate [4]. However, new boron delivery agents are currently under investigation [5, 6].

The BNCT has been clinically tested mainly on patients diagnosed with highly malignant glioblastomas [7–9] and persistent head and neck tumors [4, 10, 11]. Yanch *et al.* [12] performed simulations with cylindrical and elliptical phantoms to determine the optimal neutron energy for BCNT at neutron energies ranging between 0.025 eV and 800 keV. The results of this study compared two homogenous phantom situations: one representing healthy tissue (3 μg/g of ^{10}B) and the other simulation for an entire ellipsoid containing (30 μg/g of ^{10}B). These simulations did not take into account the tumor position (deep- or shallow seated), which may give rise to self-shielding by the boron before the tumor. Bisceglie *et al.* [13] reported an optimum value of the neutron energy slightly exceeding 10 keV by using the Monte Carlo N-Particle (MCNP) Transport Code for a known neutron spectrum and a deep-seated tumor.

Although there are recommendations for the neutron energy ranges cited in the International Atomic Energy Agency IAEA-TECDOC-1223 [14], these are based mainly on the experience gained from using the research reactor BNCT facilities and involve adjusting the epithermal flux (0.5 eV < E < 10 keV) to approximately 10^9 n/cm^2/s and minimizing the dose from gamma rays and fast neutrons.

The use of neutron sources such as pulsed neutron generators minimizes the gamma-ray source and screen the undesirable high-energy neutrons using filters. Moreover, using neutron sources allows sending well-determined pulses in different directions according to a specific treatment plan. This treatment plan takes into consideration the position of the tumor and the suitable neutron energy spectrum corresponding to tumor depth. Unlike research reactors, neutron generators can be easily installed in hospitals and can be switched off after use, thereby reducing the operating time and radiation exposure to both patients and workers. Using neutron generators requires moderating the neutrons to a suitable energy spectrum that is appropriate to the tumor depth. Depending on the tumor sitting and the different reaction types separately at discrete neutron energies, the main objective of this work is to determine the optimum neutron energy spectrum to maximize the neutron dose to the tumor and minimize the exposure at the surrounding healthy brain tissues.

2. Radiobiology Considerations

The BNCT comprises a two-step sequence in which a delivery tumor-seeking agent containing ^{10}B is initially administered to the patient. This radio-sensitizer is largely taken up in the neoplastic cancer cells compared to healthy cells owing to their faster metabolism [15]. Following the uptake, the patient is irradiated with a high-fluence neutron beam of appropriate energy. Owing to its high cross-section for thermal neutrons (3840 barns at 0.025 eV), the ^{10}B undergoes a nuclear reaction producing an α-particle and a recoiling ^{7}Li nucleus. The two fragments release their kinetic energy inside the neoplastic cells. Further, the BNCT involves

other radiation, namely γ-photons from the neutron capture reaction $^{1}H(n,\gamma)^{2}H$, protons from the $^{14}N(n,p)^{14}C$ reaction, and fast neutrons from elastic scattering.

The absorbed dose in healthy and tumor tissues is the sum of four dose components with different linear energy transfers (LETs) and different relative biological effectiveness (RBE) as stated below:

- boron dose from the products of $^{10}B(n,\alpha)^{7}Li$ reaction,
- γ-dose from the neutron capture reaction $^{1}H(n,\gamma)^{2}H$,
- proton dose from the $^{14}N(n,p)^{14}C$ reaction,
- fast neutron dose from the elastic scattering reaction.

Table 1. RBE values for radiation types and tissues involved in the BNCT [16]

Type of reaction	Energy (MeV)	Relative biological effectiveness (*RBE*) in			
		Skull	Skin	Healthy tissue	Tumor
$^{10}B(n,\alpha)^{7}Li$	E_α = 1.47 E_{Li} = 0.84	1.3	2.5	1.3	3.8
$^{1}H(n,\gamma)^{2}H$	E_γ = 2.22	1	1	1	1
$^{14}N(n,p)^{14}C$	E_p = 0.626	3.2	3.2	3.2	3.2
$^{1}H(n,n)^{1}H$	$E_p = E_n/2$	3.2	3.2	3.2	3.2

In this work, three assumptions are considered in the dose calculation:

- All charged and non-charged particles travel in straight lines,
- the ^{10}B atoms are uniformly distributed in the boron-containing media (healthy and tumor tissues),
- the same range is used for both the boron-containing healthy and tumor tissues.

The total equivalent dose rate per interaction in both the tumor tissues and surrounding healthy tissues due to the different BNCT radiation components are determined separately.

Hydrogen (H) and nitrogen (N) are present in relatively high concentrations that they contribute significantly to the total radiation absorbed dose, as shown in Eq. (1).

$$D_{tot} = D_\gamma + D_B + D_n + D_p \quad (1)$$

where:

D_γ is the dose from the gamma-rays generated by the reaction $^{1}H(n,\gamma)^{2}H$,

D_B is the dose from the capture of a thermal neutron by the boron in the reaction $^{10}B(n,\alpha)^{7}Li$,

D_n is the dose from the elastic scattering by hydrogen in the reaction $^{1}H(n,n)^{1}H$, and

D_p is the dose from the neutron capture by nitrogen in the reaction $^{14}N(n,p)^{14}C$.

The absorbed dose is computed as

$$D_i = N \times E_i \quad (2)$$

where:

N is the number of interactions per unit volume and

E_i is the energy of the reaction i.

The RBE and energies of the four doses components in different tissue types are shown in Table 1.

3. Methodology

To optimize the performance of the BNCT technique in curing brain tumors, there are two main targets: (i) maximizing the dose at the tumor tissues, and (ii) minimizing the dose at the healthy brain tissues to avoid the risk of secondary cancer induction. In all cases, the incident neutrons penetrate the skin, skull, healthy tissues, and tumor tissues.

Although the $^{10}B(n,\alpha)^{7}Li$ reaction has $1/v$ cross-sections, which imply that thermal neutrons have a higher probability of initiating the reaction, deep-brain tumors require more energetic neutrons to penetrate

healthy tissues and reach the malignant tumor.

All the neutron reactions with different tissues must be examined for accurate dose estimation in healthy and tumor cells. The MCNP has the capability to tally every interaction type distinctly, thus enabling the estimation of its effect on different tissues and its contribution to the total received dose.

A record of the results per neutron per second facilitates investigation of the effect of neutron energies independent of the source strengths or exposure times. Further, it facilitates the design of moderators and filters for different source spectra and strengths if the required optimum energy is known for a certain tumor depth. A variation in the thickness of the moderator or filters helps to design a more adjustable facility for different tumor depths.

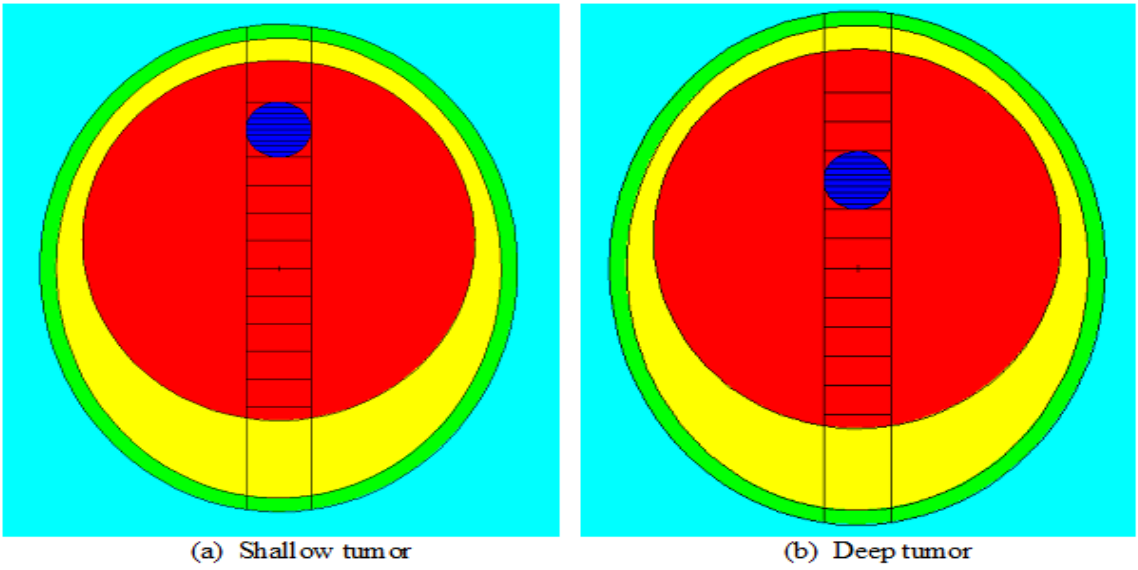

Fig. 1 MCNP geometry model for brain tumors (a) shallow-seated from 3–5 cm (b) deep-seated from 5–7 cm.

Neutron generators and accelerator-based neutron sources provide pulses of neutrons with high intensities up to 1012 n/cm^2/s that can be switched on and off after a suitable exposure time. Neutron filters help to shape the neutron energy spectrum to the desired values. To investigate the effect of the incident neutron energy on the dose received by healthy brain tissues and tumor tissues, two MCNP models are constructed to represent shallow and deep tumors. The shallow tumor is located 1 cm away from the inner surface of the skull, whereas the deep tumor is located 3 cm from the same surface. The tumor is represented by a sphere of radius 1 cm that is divided into 10 cells of thickness 2 mm each, as shown in Fig. 1.

4. Results and Discussion

The total dose was calculated for deep- and shallow-seated tumors, for incident neutron energies ranging from 0 eV to 100 keV. The ICRU 46 [17] material compositions of skin, skull, healthy tissues, and tumor tissues are used in this work. Boron concentrations in both healthy and tumor tissues are 19 ppm and 65 ppm, respectively [18, 19]. The neutron source is a disk of radius 1 cm located on the outer surface of the skin. The energies of the source are classified into three groups: 0 to 0.1 keV, 0.1 keV to 1 keV in steps of 0.1 keV, and 10 keV to 100 keV in steps of 10 keV.

The four main types of interactions namely, ^{1}H(n,γ)^{2}H, ^{14}N(n,p)^{14}C, ^{1}H(n,n)^{1}H, and ^{10}B(n,α)^{7}Li are tallied using reactions 102, 103, 2–4, and 107 respectively in the MCNP. Tally multipliers are used to determine the total interactions per cm^3 per second per neutron for each reaction type.

results for deep-seated tumors show that, at the same neutron energy, a higher dose is delivered to the healthy cells than to the tumor (Fig. 2).

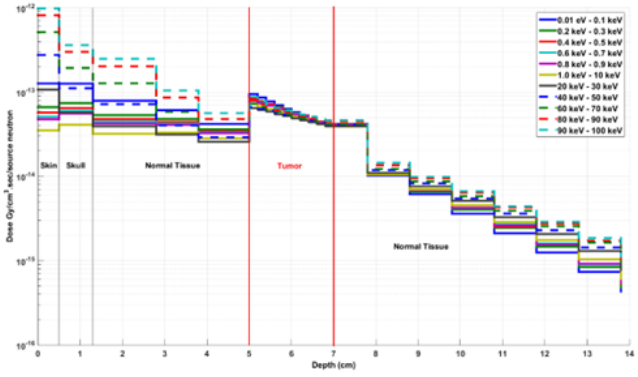

Fig. 2 Dose rate (Gy/s per neutron) to deep-seated tumors for different neutron energy groups.

This is undesirable in radiotherapy treatment, where the objective is to destroy the tumor cells rather than the healthy ones. Consequently, more effective neutron energies

must be selected that maximize the dose to the tumor cells while minimizing it to healthy cells.

The total dose delivered to the malignant tumors is between 4E-14 and 9E-14 Gy/s per neutron. The range for skin is the widest, from 3E-14 to 1E-12 Gy/s per neutron, and that for the skull is 3E-14 to 5E-13 Gy/s per neutron. Healthy cells preceding the tumor have a different absorbed dose, depending on their distance from the tumor, ranging from 2E-14 to 4E-13 Gy/s per neutron, and the ratio of the tumor to tissue dose is 0.895 in this case. These results show that the more energetic neutrons with energies ranging from approximately 20 keV to 100 keV delivered higher doses to the skin, skull, or healthy tissues preceding the tumor than to the malignant tumor itself, as seen in Fig. 3. Neutrons in the lowest energy group exhibited the same effect with higher doses delivered to the skin and skull.

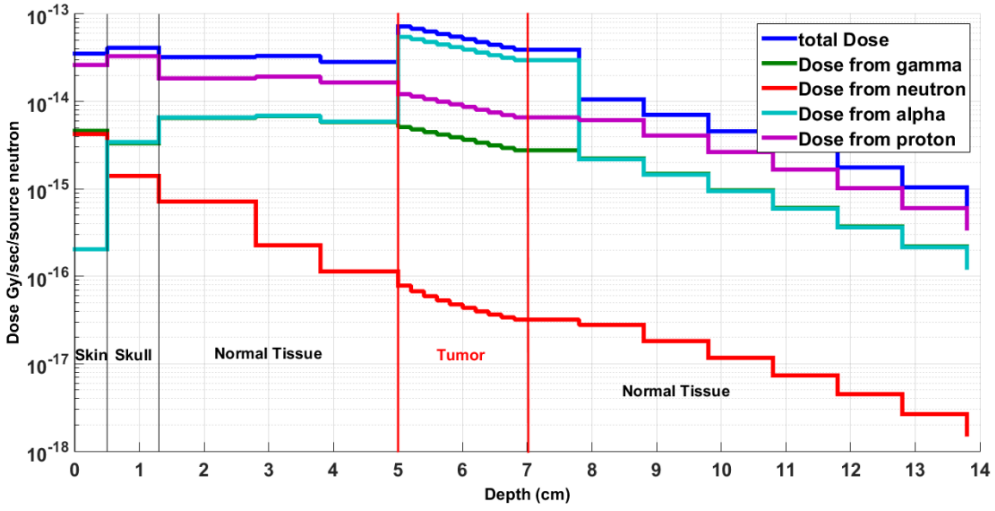

Fig. 3 Total dose rates (Gy/s per neutron) deposited in deep-seated tumors by different reactions for select neutron energy range (10–20 keV)

A review of the dose contributions of the four neutron reactions showed that the neutrons in the energy range of 10–20 keV are the most efficient at delivering higher dose ratios to the malignant tumor compared to healthy tissues preceding the tumor, as shown in Fig. 3.

Using this selected energy group, an average total dose rate of 5.16E-14 Gy/s per neutron can be delivered to the malignant tumor, compared to 6.94E-12 Gy/s per neutron that can be delivered using the full neutron energy spectrum recommended by the IAEA - TECDOC-1223, as shown in Fig. 3.

The absorbed dose in healthy cells preceding the tumor is centered on 3E-14 Gy/s per neutron, which represents a substantial reduction from the original dose of 7.76E-12 Gy/s per neutron received, using the IAEA recommended spectrum. In this model, the dose delivered to the tumor cells is 1.8 times

higher than that delivered to the healthy cells preceding the tumor, and 12 times higher than that delivered to the healthy cells after the tumor.

The major contributor to this undesirable dose in the three regions preceding the tumor is the energy deposited by the protons, which are produced by neutron interactions with nitrogen. The presence of nitrogen (^{14}N) in the human body remains the main cause of this dose contribution, which can be reduced only by selecting neutron energies with low microscopic cross-sections.

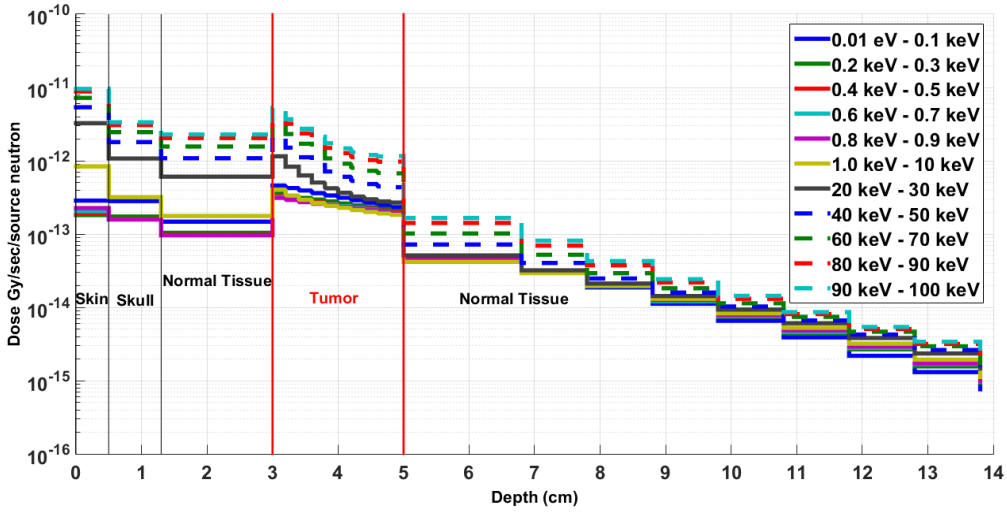

Fig. 4 Total doses (Gy/s per neutron) deposited in shallow tumors at different neutron energy groups

The results show that, in general, a higher dose is delivered to the shallow-seated tumors than the deep-seated tumors, as seen in Fig. 4. A comparison of the results shown in Figs. 2 and 4 indicates a difference of one order of magnitude between the maximum doses delivered to the tumors in both cases.

Table 2 shows that for neutron energies based on the IAEA recommendation, the dose rate per volume is received by the skin at 6.18E-12 Gy/s per neutron. The tumor dose is as high as 5.73E-12 Gy/s per neutron, whereas it is 3.3E-12 Gy/s per neutron in the skull. The dose delivered to healthy cells remains relatively high at 2.31E-12 Gy/s for the cells preceding the tumor and 6.64E-13 Gy/s per neutron for the cells past the tumor.

A review of the dose contributions of the four neutron reactions showed that neutrons in the energy group of 0.3–0.4 keV are the most efficient at delivering high doses to the malignant tumor, while reducing that to the healthy ones, with a ratio of 2.64 and 18.8 for tumor to soft tissues before and after the tumor, respectively.

The total doses delivered to the skin and skull are 1.84E-13, and 1.65E-13 Gy/s per neutron, respectively, which is approximately one order of magnitude lower than that received by the skin, using the IAEA recommended spectrum.

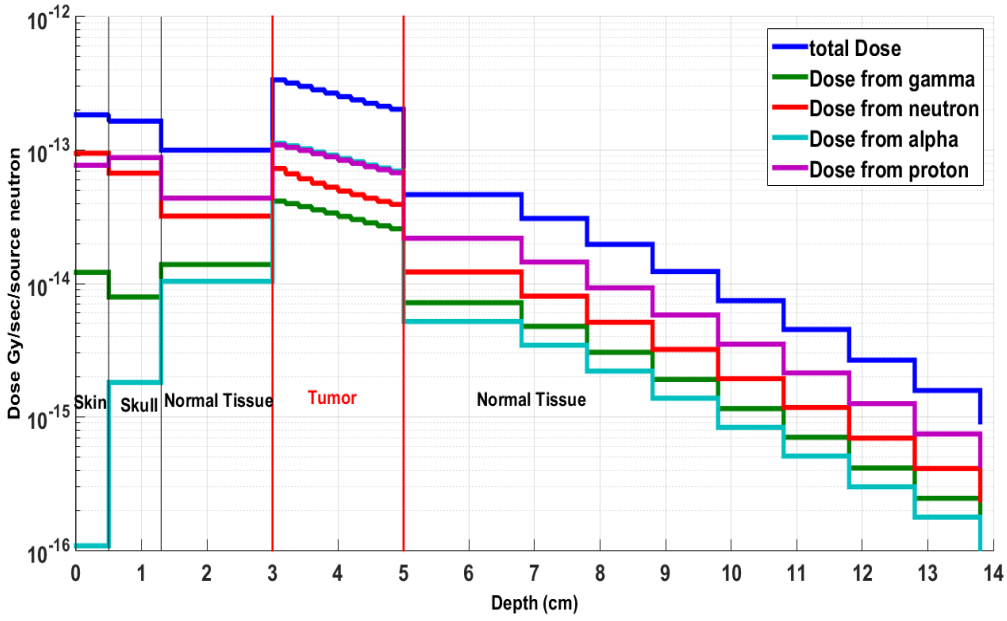

Fig. 5 Total dose rates (Gy/s per neutron) deposited in shallow-seated tumors by different reactions for selected neutron energy range (0.3–0.4 keV).

The results shown in Fig. 5 indicate a vast reduction in the dose received by healthy brain cells. The absorbed dose in healthy cells preceding the tumor is reduced by order of magnitude from 2.31E-12 to 1.0E-13 Gy/s per neutron, whereas that in healthy cells after the tumor is reduced from 6.6E-13 to 1.4E-14 Gy/s per neutron. The total dose delivered to the tumor cells is approximately three times higher than that received by the soft brain tissues. It is also observed that the dose due to α- particles are almost equal to that from protons for the shallow tumors, whereas it is one order of magnitude higher than the proton dose in the deep tumors.

The ratio of the dose rate deposited in the tumor cells compared to that in the healthy brain cells increases from 2.48 to 2.64 for cells located before the tumor, and from 8.6 to 18.8 for cells located after the tumor. A large improvement in the dose delivery to the malignant tumor, with reduced damage to soft brain cells, is evident.

Table 2 The average dose rate (Gy/s per neutron) for a brain tumor and surrounding healthy cells, as calculated by this work vs. IAEA BNCT recommended energies.

	Deep-Seated Dose (Gy/s per neutron)		Shallow-Seated Dose (Gy/s per neutron)	
	IAEA	Present work	IAEA	Present work
Skin	1.84E-11	5.61E-14	6.18E-12	1.84E-13
Skull	1.13E-11	4.26E-14	3.13E-12	1.65E-13
Soft Tissue before	7.76E-12	2.92E-14	2.31E-12	1.00E-13
Tumor	6.94E-12	5.16E-14	5.73E-12	2.64E-13
Soft Tissue after	2.90E-12	4.29E-15	6.64E-13	1.40E-14
Ratio TU/STb	0.89	1.77	2.48	2.64
Ratio TU/STa	2.40	12.0	8.63	18.8

The drawback of the model is that the dose rate in the tumor is also reduced from 5.7E-12 Gy/s per neutron to 2.64E-13 Gy/s per neutron; however, this can be overcome by increasing the irradiation time. Table 2 shows a comparison between the recommended neutron energies by IAEA and the results of the current MCNP model. The ratio of the dose received by the tumor to that by the soft tissues preceding it is designated as (Tu/STb); and the ratio of the dose received by the tumor to that by the soft tissues after it is designated as (Tu/STa) in Table 2.

5. Conclusion

The main objective of this study was to construct a methodology to determine the optimum neutron energy according to the depth of the tumor. This methodology depended mainly on calculating the different types of reactions separately for discrete neutron energies. For a certain tumor depth, the neutron energy was selected to maximize the neutron dose at the tumor and minimize the risk of secondary tumors at the healthy brain tissues. This was accomplished by specifically calculating the ratio of the dose rate density delivered to the tumor to that delivered to the healthy brain tissues. For deep-seated tumors, the optimum energy was determined to be 10–20 keV and at this energy, the ratio of the dose rate of the tumor to that of healthy brain tissues improved from 0.89 to 1.77 for cells preceding the tumor, and 2.4 to 12 for cells located after the tumor. For shallow-seated tumors, the optimum energy was determined to be 0.3–0.4 keV. At this energy, the ratio of the dose rate of the tumor to that of healthy brain tissues improved from 2.48 to 2.64 for cells preceding the tumor, and from 8.63 to 18.8 for cells located after the tumor. In both cases, the selection of the optimum energy maximized neutron doses to the tumors and minimized them to healthy brain tissues, thus reducing the risk of secondary tumors in the surrounding healthy brain tissues.

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دراسة الطيف الأمثل لطاقة النيوترون في علاج ورم الدماغ بطريقة إلتقاط النيوترون بالبورون باستخدام طريقة مونت كارلو لانتقال الجسيمات

عبدالفتاح سليمان، عصام بانقيطة، نضال الزغبي، وفتحي جويدر

مستخلص. يعتمد علاج التقاط البورون النيوتروني ، وهو أسلوب موجه لعلاج السرطان ، على التفاعل الانشطاري للبورون ١٠ المزروع في الخلايا السرطانية بواسطة النيوترونات الحرارية لإنتاج جسيمات ألفا ونواة الليثيوم - ٧ المرتدة. يتسبب المدى القصير لمنتجات الانشطار المؤين في إتلاف الخلايا السرطانية مع الحفاظ على الأنسجة السليمة المحيطة. تم تطوير منهجية لتحديد الطاقات النيوترونية المثلى وفقًا لعمق الورم في المخ في هذا العمل. تعتمد هذه المنهجية بشكل أساسي على حساب أنواع التفاعلات المختلفة بشكل منفصل في طاقات النيوترونات المنفصلة باستخدام كود إنتقال الإشعاع بطريقة مونت كارلو والتحقيق في مساهمتها النسبية في الجرعة الممتصة في كل من الورم والأنسجة السليمة المحيطة. للحصول على عمق معين للورم ، يتم اختيار طاقة النيوترون التي تزيد من جرعة النيوترون إلى الحد الأقصى وتقليلها في الأنسجة السليمة المحيطة بها. يتم تطوير المقاييس لتقييم التحسن في عملية التحسين بناءً على نسبة كثافة معدل جرعة الورم ($Gy / cm^3 \cdot s$) إلى نسبة الأنسجة السليمة المحيطة. أظهرت النتائج تحسنا كبيرا بالمقارنة مع تلك التي أوصت بها الوكالة الدولية للطاقة الذرية نطاقات الطاقة النيوترونية. بالنسبة للأورام العميقة الجذور، تحسنت نسبة الجرعة من ٠,٨٩ إلى ١,٧٧ للأنسجة التي تسبق الورم ومن ٢,٤٠ إلى ١٢,٠ للأنسجة بعد الورم. في الحالات الضحلة، تحسنت نسبة الجرعة من ٢,٤٨ إلى ٢,٦٤ للأنسجة السابقة للورم ومن ٨,٦٣ إلى ١٨,٨ للأنسجة بعد الورم.