Monte-Carlo Simulation for Beam Shaping Assembly of Boron Neutron Capture Therapy

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Abstract

Many researches in the BNCT including clinical trials and theoretical simulations for both beam shaping assembly and its corresponding dosimetry were carried out, especially in the past decades. Major aim of the present study is beam shaping assembly of a D-T neutron source to make epi-thermal neutrons for BNCT. Therefore, Monte-Carlo simulations for beam shaping of a D-T neutron source are carried out using MCNP5 code.

Keywords
BNCT; D-T neutron source; Epi-thermal; MCNP5.

1. Introduction

Boron Neutron Capture Therapy (BNCT) early proposed as a treatment modality for deeply-seated brain cancer-tumors so that surgery does not possible and/or makes high risk. But its neutron beam design energy optimization and corresponding treatment are difficult depends on tumor depth, size, kinds of tumor, and therefore varies for each patient. So far, many researches are made, especially in the recent decade, for both optimum neutron sources and best beam shaping assemblies [e.g, Riley et al., 2008; Blue and Yanch, 2003; Hatanaka, 1990; Brugger et al., 1992]. Moreover, BNCT has been clinically used to treat a variety of cancers at various sites worldwide: in the USA [Chanana et al., 1999; Palmer et al., 2002; Busse et al., 2003; Kiger III et al., 2004] in Japan [Kato et al., 2004; Yamamoto et al., 2004] in Europe [Vos et al., 2005; Burian et al., 2002; Joensuu et al., 2003; Capala et al., 2003; Zonta et al., 2006] and in Argentina [González , 2004]. A major concern and inquiry arises as ``can we design a Neutron Beam Shaping Assembly (NBSA) that be adjusted for each patient"? To answer we say, NBSA depends on the tumor's depth and size (also kinds), and it is major difficulty concern of BNCT. Obviously, due to tumor location and its size and type, patient age, and other clinical problems we should use different NBSA (for the fast neutrons) for each patient with different moderator/reflector and filter size to obtain epi-thernal beam. Therefore, BNCT and its NBSA should be varied due to patient clinical diagnose and hence this type of treatment is so complicated and involves a team-working between health physicists and medicine doctors. B-10 has a high *thermal* neutron capture cross section of 3840b. If the tumor is collated on the skin surface, a thermal neutron beam can be used directly. However, if the tumor is located at depth below the skin surface, epi-thermal neutron beam is needed. This relies on the neutron losing energy by elastic scattering with brain tissue and becoming thermalized by the time they reach the tumor. The advantage depth is defined as the depth at which the total dose delivered to the tumor equals the maximum dose delivered to healthy tissue. Based on our Monte-Carlo simulations, which are described later, results in neutron energy of 4eV-40KeV needed for a 2-3cm depth tumor, which is approximately half-distance from the surface to the middle of an adult brain. For neuron energy of more than 40KeV, proton reaction (a side-reaction) increases and for neutron energy of below 4eV neutron do not penetrate to the deeply- seated tumor. In this article two aims are studied. First, a proposed structure is investigated and also simulated to get the best NBSA for 3 cm seated tumor, and also for a D-T neutron source. Secondly, the percent depth dose calculations in the Snyder head phantom are given. All neutron transports are carried out using MCNP5 code [X-5 Monte Carlo Team, 2003].

2. Neutron Beam Shaping Assembly of a D-T Source

Briefly, useful and hospitality source for BNCT are accelerator-based neutron sources such as proton beam of 2.4MeV (fluence proportional to 20-50mA current) which is followed $^{7}Li\,(p,n)^{8}Be$ reaction, and proton beam of 4.1MeV (fluence proportional to 20-50mA) which is followed for instance $^{9}Be(p,n)^{8}B$ reaction. Therefore, high energy accelerator is required. Table 1 contains a comparison between parameters of some more familiar accelerators and the BMRR (3MW Brookhaven Medical Research Reactor) which produce epi-thermal neutron sources (after moderation), can be used in the BNCT.

Table 1: Comparison of accelerators and the BMRR which produce epi-thermal neutron beam (for treatment planning via BNCT) using different moderator [Green, 1998; Vujic, 2003]

Parameter	**BMRR**	$^{7}Li\,(p,n)^{8}Be$	$^{7}Li\,(p,n)^{8}Be$	$^{7}Li\,(p,n)^{8}Be$
Moderator, thickness (cm)	Al_2O_3	Al(40%)+AlF_3 (60%),34	LiF, 22	D_2O, 17
Proton energy (MeV)	-	2.4	2.3	2.2
Proton current (mA)	-	20	20	20
Treatment time (min)	39	54	40	45
Tumor dose (max) (Gy-Eq)	61.6	65.6	64.3	62.3
Tumor dose (5cm) (Gy-Eq)	38.6	51.4	50.5	39.1
Tumor dose (8cm)(Gy-Eq)	14.5	22.3	21.4	16.1

Another useful neutron source is a fission converter-based (coupled with a moderator) epi-thermal neutron beam which has been used in clinical trials of BNCT [e.g., Kiger III et al., 2004] that have been well-validated against physical measurements made in an ellipsoidal head phantom which is out of the scope of the present research. Moreover, a D-T fusion-based accelerator is another choice which is taken in this study and its scheme are given in Figure 1. In this case, we need to accelerate deuterium beam up to 120KeV which causes local fusion with tritium target and hence emits 14.1MeV neutrons. For NBSA of the D-T neutron source, the goal here is to produce epi-thermal neutron beam with optimal characteristic that can deliver maximum dose to a 3-4 cm seated-tumor with minimal exposure to healthy tissue. Therefore, we need to thermalize high energy neutrons using a fine moderator/reflector/filter set-up.

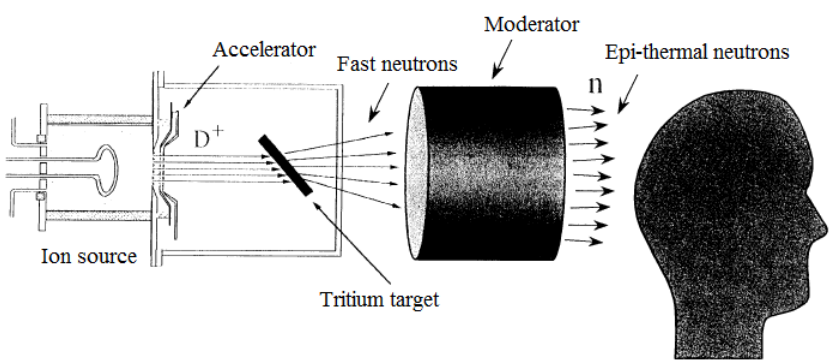

Figure 1: A simple scheme set up for the D-T based neutron beam and neutronic thermalization to obtain epithermal (4eV-40Kev) beam

2.1 Monte-Carlo simulation

First, it is constructive to estimate neutron flux for D-T accelerator with very large deuterium current of 1A: $q = ne = n \times 1.6 \times 10^{-19} = it = 1 \times t$. For a 120keV deuteron kinetic energy (velocity ~3.4×$10^{6} m/s$) the flight time of deuterons (between anode-cathode) are 0.29×$10^{-6} s$. Therefore, the numbers of deuterons are equal to 1.8×10^{12} *deuterons*. As a result of one-by-one deuterium-neutron production regarding to $d + t \rightarrow n + \alpha$ reaction, there are equal fast neutrons for each incident deuterium. But, the reaction efficiency is equal to (at most) 0.01 so that the neutron numbers are about 1.8×10^{10} *neutrons*. Our simulated tritium target disc (as shown in Figure 2 and also is given in the Appendix) has 17.5cm radius, and therefore the emitted *neutron fluence* is estimated to be

$1.8 \times 10^{10} / \pi \times 17.5^2 = 1.9 \times 10^7\ neutrons / cm^2$. Finally, the neutron flux of a D-T accelerator (current=1A & deuterium energy=120 keV) is estimated to be $6.5 \times 10^{13}\ neutrons / cm^2.s$ which is a huge flux for an accelerator. In our Monte-Carlo simulation, using MCNP5 code, instead of source simulation, we have considered a cylinder of 17.5cm radius and 1 cm thickness (approximately considered as an infinite planner source) which emits $6.5 \times 10^{13}\ neutrons / cm^2.s$ of 14.1MeV energy in a mono-direction. Obviously, for a smaller tritium target (kathode), the mentioned mono-directional infinite planner source does not a good approximation. Figure 2 shows a proposed beam shaping assembly [Verbeke et al., 1998] including moderator, reflector, and filter to obtain 4eV-40KeV output neutrons from the above suggested D-T source.

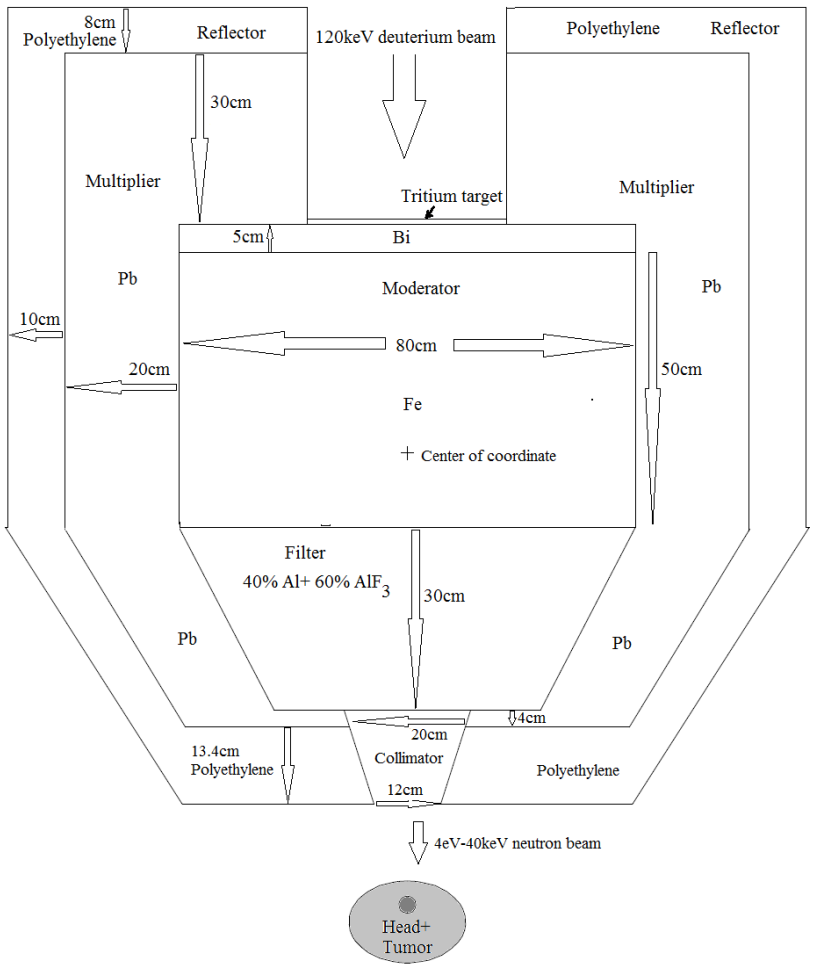

Figure 2: Cross sectional view of the beam shaping assembly.

Based on the proposed beam shaping assembly (Figure 2) and MCNP5 execution (considering the above source estimation in the SDEF) and the following criteria, we have optimized the structure to slow-down neutrons into 4eV-40keV epi-thermal beam. The physics for considering each part of the assembly and also their dimensions are as follow:

2.1.1 Internal multiplier

This layer is considered to increase neutron flux based on *(n, 2n)* and *(n, 3n)* reactions in the fast region. We have chosen and examined three materials Bi, U, and Pb which contain acceptable *(n, 2n)* cross section for 14MeV neutrons. We have run MCNP5 (based on Table 2 data) including different materials and variable thickness and found neutron current (F1 tally) and also neutron flux in the each cell (F4 tally), which are given in Figs. 3. Based on

Figs. 3, Bi of 5cm thickness is the best choice as the multiplier region. Our constraint here, for choosing the best material, has been that "number of neutrons in the material should be greater than that initial supposed number of particles (histories) together with most current to flux ratio". In another words, based on the MCNP notations, F4 tally in each cell should be greater than the supposed NPS together with most $\frac{current}{flux}$ ratio. Lead (Pb) is still another good choice as neutron multiplier, but due to gamma emitting, we have not recommended U as a multiplier. Recently, U was considered as a wrong material in some literatures [e.g., Rasouli et al., 2012] to use its fast fission reactions and therefore its corresponding neutrons without considering its harmful gamma emissions due to its radiative capture cross section.

Table 2: $\sigma_{(n,2n)}$ cross section at 14MeV for our used materials as multiplier

Material	Density (g/cm^3)	$\sigma_{(n,2n)}$ at 14MeV (b)
Pb	11.34	2.04
U	19.1	2.15
Bi	9.74	2.14

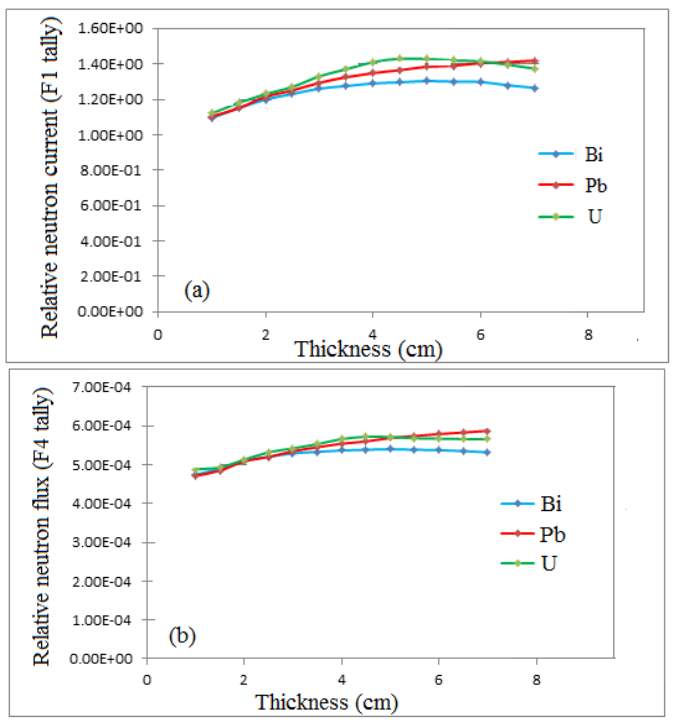

Figure 3: Neutron flux as well as current in three suggested multiplier adjacent to the source

2.1.2 Moderator

A moderator should contain less atomic mass, less absorption cross section and most scattering cross section (in another words a good moderating ratio is found based on M.R= $\xi \Sigma_{scattering} / \Sigma_{absorption}$). Moreover, in the BNCT, we need a moderator includes less radiative capture cross section (n,γ), and less gamma emission in the inelastic collisions to avoid harmful gamma for patient. At a glance, very Light nuclei are the first choice but due to their huge gamma emissions regarding (n,γ) reaction, we have neglected these nuclei as a moderator for BNCT. In the recent literatures, Fluental (a mixture of 1% LiF+30% Al+69%AlF) is also proposed [Verbeke et al., 1998], but Fluental is suggested as the ''filter'' in the next part of the present NBSA. Medium materials such as Fluental, Fe, Al, Ni, AlF_3, Al+AlF3, and LiF which are approximately satisfied the above mentioned criteria were proposed as a

good moderator for BNCT [Verbeke et al., 1998]. We have examined these materials and compute $\frac{\varphi_{epi-thermal}}{\varphi_{fast}}$ versus moderator thickness. Obviously, we desire to have more $\frac{\varphi_{epi-thermal}}{\varphi_{fast}}$ in the optimized thickness. As we said before, a good moderator for BNCT should not include effective (n,γ) reaction so that we select a material which contains less gamma dose rate. Therefore, for our purpose, we should compute $\frac{\dot{D}_{\gamma}}{\varphi_{epi-thermal}}$ versus moderator thickness. Using F1, F2, F6, and F8* tallies for mentioned materials and for NPS=2×10^{10}(this is upper than that the estimated neutron number of 1.8×10^{10}), and calibration the output results, Figs. 4 are obtained. The optimized thickness are chosen so that $\frac{\dot{D}_{\gamma}}{\varphi_{epi-thermal}}$ <2×10^{-13}, and $\frac{Current}{Flux} > 0.7$ [IAEA-TECDOC-1213, 2001]. Based on Figure 4 results and the mentioned IAEA optimization criteria, we have verified that Fe with 50cm length and 80 cm thickness is the optimized choice for considering as the moderator material (c.f., Figure 2). Obviously, Fe is the cheapest one and more abundant in comparison with other mentioned materials especially Fluental.

2.1.3 Filter

Filter is chosen to more increase $\frac{\varphi_{epi-thermal}}{\varphi_{thermal}}$ as well as $\frac{\varphi_{epi-thermal}}{\varphi_{fast}}$. So, we need materials to contain low epi-thermal neutron absorption cross sections as well as high thermal absorption cross section. Another constraint is also less radiation capture cross section. We studied many materials as the filter (but have plotted our results for the best choices, c.f. Figure 5). Based on the practical IAEA report [IAEA-TECDOC-1213, 2001], we have optimized the filter dimensions according to $\frac{\varphi_{epi-thermal}}{\varphi_{thermal}} > 100$ and $\frac{\varphi_{epi-thermal}}{\varphi_{fast}}$>20, we have recommend Al(40%)+AlF_3(60%) as the suggested filter so that its dimensions are given in the Figure 2.

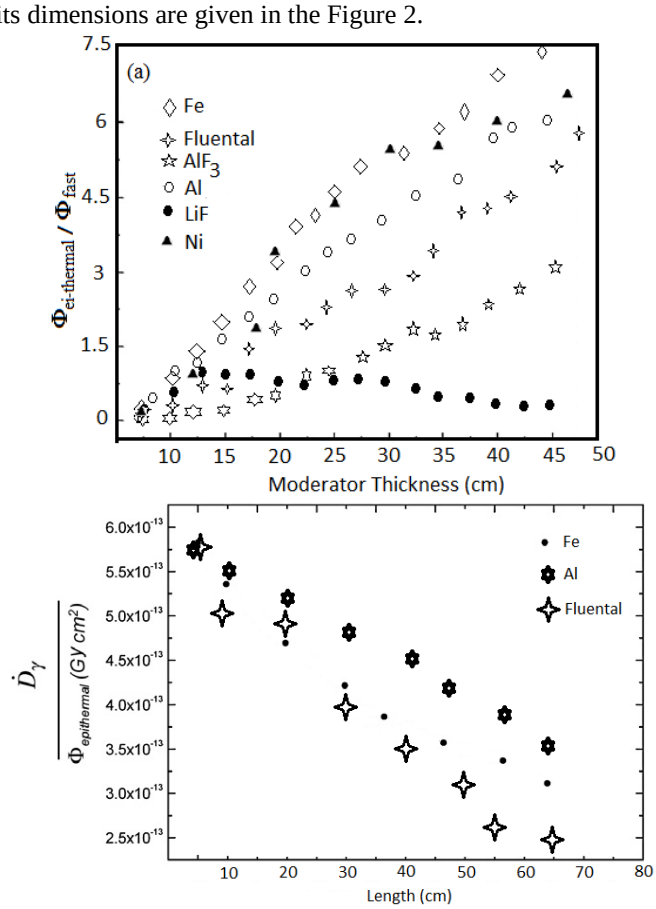

Figure 4: (a) $\frac{\varphi_{epi-thermal}}{\varphi_{fast}}$ and $\frac{\dot{D}_{\gamma}}{\varphi_{epi-thermal}}$ are two constraints for choosing the best moderator.

2.1.4 External multiplier

Consider an egg including yolk and white which is surrounded by a shell. If we suppose Figure 2 as an egg, the moderator and filter is similar to the egg's yolk and the external multiplier is like as egg's white. Therefore, reflector is same as an egg's shell. Same as the white of an egg that nutrition a yolk to make a new-born bird, the supposed external multiplier compensates neutron lossage in the moderator and filter. Physically, there are many fast neutrons which collide in the moderator (and also filter), and then scattered into external multiplier with a fewer energy (but still they are fast neutrons close to ~ 10MeV). External multiplier is considered around the moderator and filter to compensate neutrons. Same as internal multiplier, Pb is suggested as the external multiplier due to its high *(n, 2n)* reaction (c.f., Figure 6), and also its optimum dimensions are given in Figure 2.

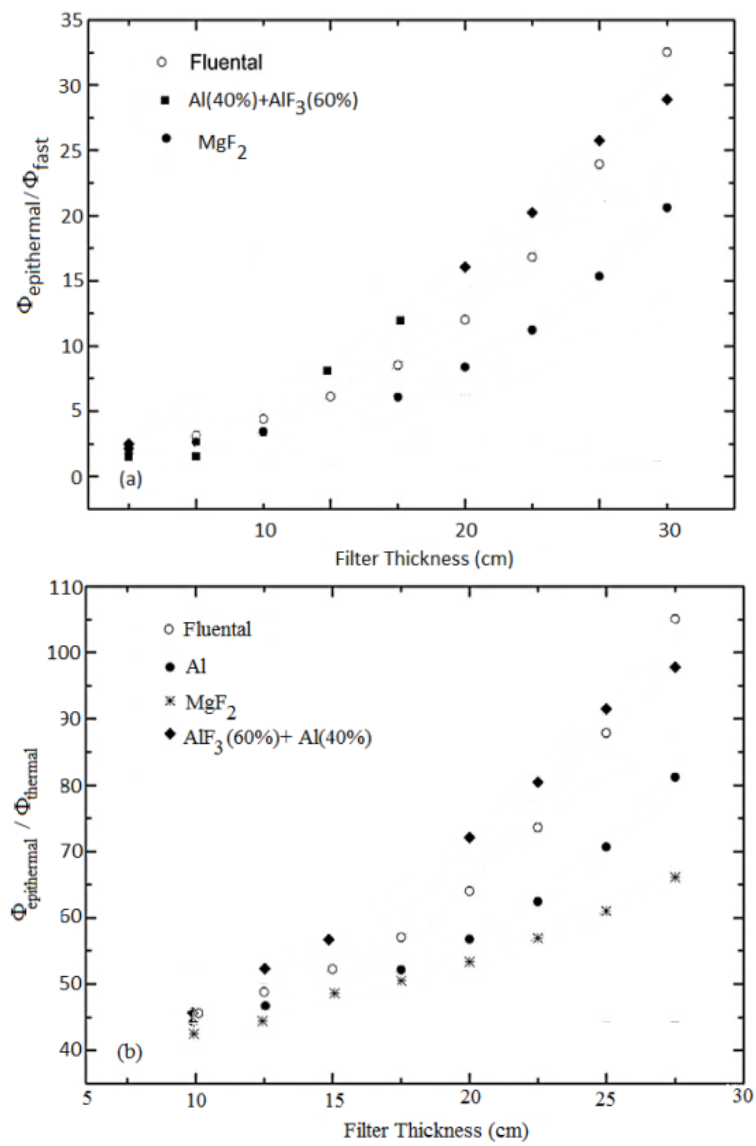

Figure 5: $\frac{\varphi_{epi-thermal}}{\varphi_{thermal}}$ and $\frac{\varphi_{epi-thermal}}{\varphi_{fast}}$ are two constraints for choosing the best filter.

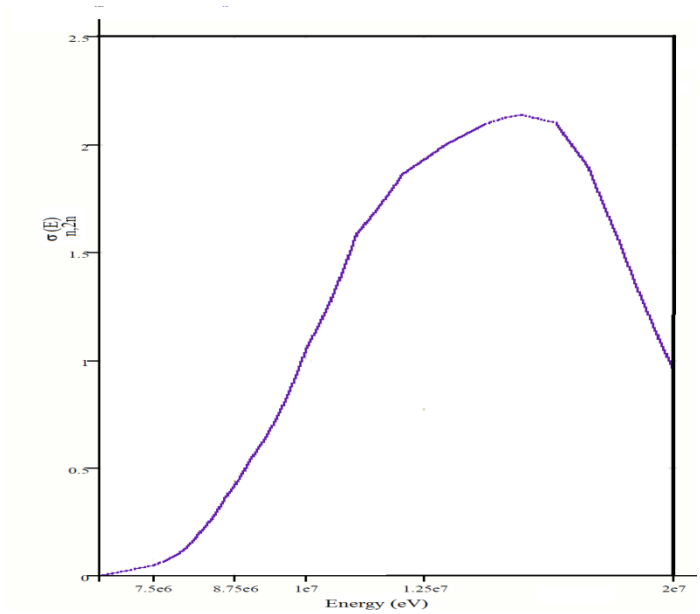

Figure 6: *(n, 2n)* cross section of the lead as a function of energy

2.1.5 Reflector

A reflector is considered to reflect neutrons into external multiplier and/or moderator regions. Our criteria for obtaining its dimensions had been its relative neutron current. In another words, we found F1 tally on the suggested reflector surface and for different dimensions which are compared with initial neutron source current. Mathematically, in our simulation, we have supposed $\frac{\text{Current on the reflector surface}}{\text{Initial current adjacent to the reflector}}$ should be less than 10^{-4}, and determined its corresponding dimension.

2.1.6 Collimator

Obviously, collimator is used to focus output neutron beam to the head phantom and its seated-tumor for better treatment planning. Reflector material (Lithium Polyethylene) is designed in a trapezoidal shape to collimate output neutron beam (c.f., Figure 2). Finally, based on the explained designing, three dimensional view of the suggested NBSA for a D-T source is given in Figure 7. Now, we should examine the output neutron beam energy of the suggested facilities (as we explained before, the neutron beam energy should be in the epi-thermal region of 4eV-40keV for BNCT).

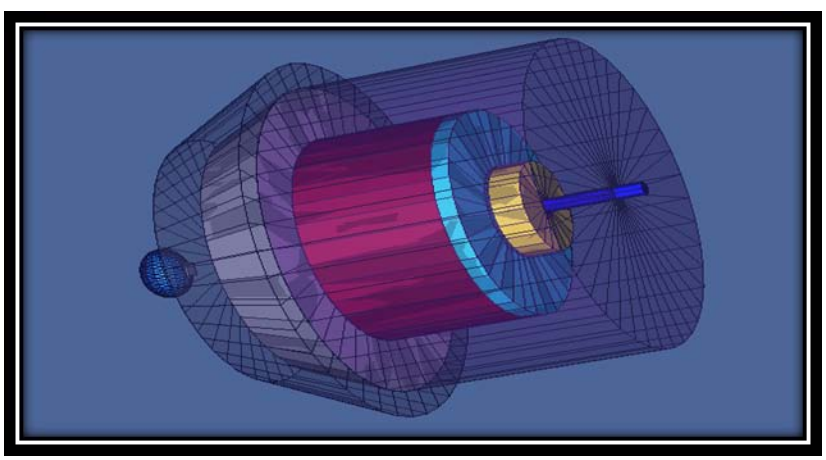

Figure 7: Three dimensional view of the examined NBSA

According to the explained NBSA and MCNP5 execution, we have plotted (Figure 8) the tally (F4: En) energy card to subdivide the flux into energy groups. This may be accomplished using a tally energy card (c.f., Appendix) which is given the neutron flux in terms of energy on the skin of the head. According to Figure 8, we can see that the output neutron beam has satisfied our desired epi-thermal neutron energy, and its maximum energy occurs around 10KeV which is the best energy for the BNCT treatment. Obviously, the epi-thermal beam is slowing down in the head phantom and would be thermal neutron at the position of seated-tumor when the desired reaction $^{10}B(n,\alpha)^{7}Li$ with thermal neutrons occurs.

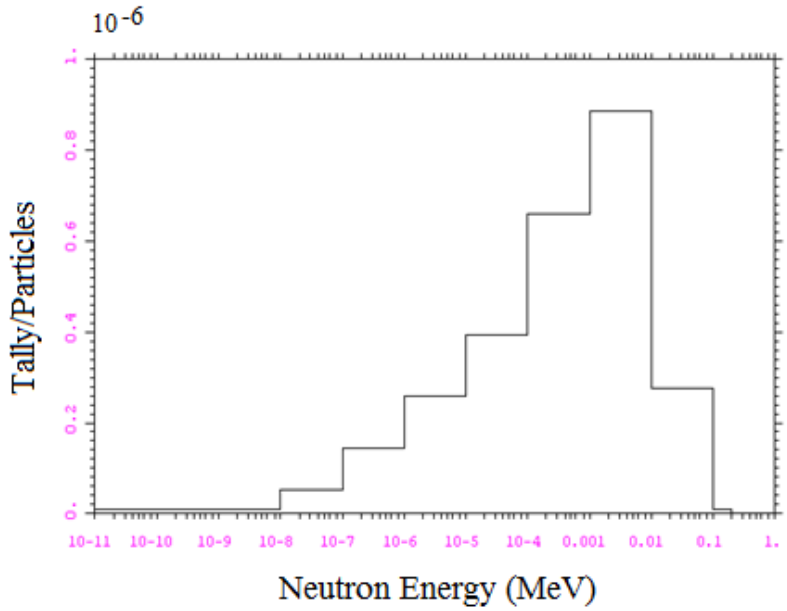

Figure 8: Output of the F4 tally energy card which is shown the neutron flux versus energy on the head skin results in the suggested NBSA.

3. Conclusions

This article describes optimization of moderator/reflector/filter assemblies to obtain epi-thermal neutron beam for the D-T fast neutron source. The second goal will be constructing an accurate description of a neutron beam to calculating corresponding doses in the BNCT planning and for deeply seated tumor in the Snder head phantom. All simulations were performed using the MCNP5 Monte Carlo radiation transport code. We believe that coupled Monte-Carlo and deterministic codes is necessary for developing BNCT in future works. Also, well understanding of the tumor geometry using CT and/or MRI images can help physicians for better therapy. Moreover, PET- based boron distribution description, as a parallel process, is another research plan for future works.

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