Neutron Moderation and Shaping for Boron Neutron Capture Therapy Using a D-Be Compact Fast Neutron Source

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Abstract

Boron neutron capture therapy is a binary radiotherapy modality with strong targeting capability at the cellular scale and high linear energy transfer, offering advantages such as short treatment cycles and minimal damage to surrounding healthy tissues, making it a promising cancer treatment modality. In BNCT devices, the beam shaping assembly serves to moderate fast neutron beams generated by the neutron source to the epithermal neutron energy range (0.5 eV < E < 10 keV) while maintaining neutron directionality. This study employs the Monte Carlo simulation codes GEANT4 and FLUKA to simulate neutron source generation from the 9Be(d,n)10B reaction and subsequent neutron moderation. Using a 1.45 MeV, 30 mA deuteron beam bombarding a 9 m thin beryllium target, neutrons produced from this reaction are used as the source term for feasibility design of the BSA. The results demonstrate that employing a 45 cm thick BiF3 and 5 cm thick TiF3 combined moderator layer, a 12 cm thick Pb reflector layer, an 11 cm thick Al2O3 supplementary moderator layer, and a 0.1 mm thick Cd thermal neutron absorber layer ensures that the gamma component, fast neutron component, Φepi/Φth, and Φepi/Φfast at the exit meet the recommended values suggested by the IAEA. This study obtains the neutron spectrum from low-energy deuteron beams and thin beryllium targets, along with a specific BSA design scheme, providing data references for neutron moderation and shaping of D-Be neutron sources and supporting further optimization research on D-Be sources.

Full Text

Design of Beam Shaping Assembly for Boron Neutron Capture Therapy Based on D-Be Compact Fast Neutron Source

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Abstract

Boron Neutron Capture Therapy (BNCT) is a binary radiation therapy with strong targeting capability and high linear energy transfer at the cellular scale, offering advantages such as short treatment cycles and minimal damage to surrounding healthy tissues, making it a promising cancer treatment modality. In BNCT facilities, the Beam Shaping Assembly (BSA) plays a crucial role in moderating fast neutrons produced by the neutron source to the epithermal energy range (0.5 eV < E < 10 keV) while maintaining beam directionality. This study employs the Monte Carlo simulation programs GEANT4 and FLUKA to simulate the 9Be(d,n)10B reaction neutron source generation and subsequent neutron moderation. Using a 1.45 MeV, 30 mA deuterium beam bombarding a 9 m thin beryllium target, the neutrons produced by this reaction serve as the source term for BSA feasibility design. The results demonstrate that two design configurations meet the recommended values of the International Atomic Energy Agency (IAEA) for gamma component, fast neutron component, Φepi/Φth, and Φepi/Φfast at the beam outlet: (1) a 45 cm thick BiF3 and 5 cm thick TiF3 combined moderating layer, 12 cm thick Pb reflector layer, 11 cm thick Al2O3 supplementary moderating layer, and 0.1 mm thick Cd thermal neutron absorption layer; and (2) a 20 cm thick BiF3 and 30 cm thick MgF2 combined moderating layer, 30 cm thick Pb reflector layer, 9 cm thick MgF2 supplementary moderating layer, and 0.2 mm thick Cd thermal neutron absorption layer. This study obtains the neutron spectrum and specific BSA design scheme for low-energy deuterium beams and thin beryllium targets, providing data reference for neutron moderation and shaping in D-Be neutron sources and supporting further optimization research.

Keywords: Boron neutron capture therapy; D-Be neutron source; Beam Shaping Assembly; Neutron moderation

1. Introduction

Neutron Capture Therapy (NCT) was first proposed by G. Locher in 1936, who noted that 10B captures a thermal neutron to produce a high-energy, short-range radioactive product with strong biological effects, suggesting that neutron capture therapy could serve as a novel cancer treatment method. Boron Neutron Capture Therapy (BNCT) offers precise tumor targeting, short treatment cycles, and minimal damage to surrounding healthy tissues, representing a promising cancer therapy. The principle of BNCT involves injecting targeted boron-containing drugs into the patient, which accumulate specifically in tumor tissue. The tumor site is then irradiated with an external beam of moderated low-energy epithermal neutrons, triggering the 10B(n,α)7Li reaction within the tumor. This reaction releases α particles and 7Li ions with ranges of approximately 10 m (about the size of a single cancer cell) and high linear energy transfer, enabling cell-level targeted killing of cancer cells while causing minimal damage to surrounding healthy tissue [?].

In 1951, W. Sweet and colleagues in the United States [?] developed a BNCT facility based on a nuclear reactor thermal neutron beam and conducted the first clinical trials. However, due to poor tumor accumulation of the boron drugs available at the time, all patients in the trial survived less than one year. In 1958, Snyder et al. [?] first synthesized boronophenylalanine (BPA). In 1987, Mishima et al. [?] in Japan applied BPA as a boron compound for BNCT treatment of malignant melanoma, achieving the first clinical application of BNCT for tumors outside the central nervous system.

Since the 1970s, research on third-generation boron drugs has emerged continuously, including boron-containing small molecules, biomacromolecules, and nanodrugs, yielding many positive results in preclinical studies. In the 1990s, MIT proposed a reactor-based epithermal neutron beam design. However, reactors suffer from large footprint, high operational costs, and potential safety hazards, limiting their clinical application and gradually leading to their replacement [?].

With advances in accelerator technology, safe, reliable, and flexible neutron sources can now be provided through radiofrequency linear acceleration, cyclotron acceleration, and high-voltage acceleration. Accelerator-based reactions studied for this purpose include 7Li(p,n)7Be, 13C(p,n)14N, 3T(d,n)4He, and 9Be(d,n)10B. Numerous organizations worldwide are actively developing accelerator-based BNCT (AB-BNCT) for clinical applications [?, ?]. In March 2020, the world’ s first accelerator-based BNCT device and the first boron drug were approved in Japan, and in May 2020, Japan announced that BNCT therapy would officially accept patients, marking the first time BNCT entered clinical application worldwide.

Domestically, China attaches great importance to BNCT technology development. In 2009, Academician Zhou Yongmu of the China Institute of Atomic Energy presided over the construction of a hospital neutron irradiator based on a miniature reactor in Beijing—the world’ s first nuclear facility dedicated to providing neutron sources for BNCT. In September 2014, this device performed China' s first clinical trial of BNCT for a melanoma patient, achieving excellent therapeutic outcomes [?]. The accelerator BNCT cancer treatment center jointly built by Zhongboron Medical and Xiamen Hong' an Hospital completed installation and successfully produced a beam in August 2021, initiating full performance testing and animal experiments to advance clinical progress. In April 2024, Ruisc Medical collaborated with Jinjiang City to present innovative technologies including a fully independent intellectual property rights accelerator-based BNCT system and precision radiotherapy systems at a technology fair, accelerating the domestic production of medical equipment in China.

Compared to the 7Li(p,n)7Be reaction, the 9Be(d,n)10B reaction offers significant advantages for stable neutron production. Metallic beryllium possesses suitable thermal and mechanical properties, with a melting point of 1287°C and thermal conductivity of 190 W/m・K, compared to lithium' s 180°C and 84.7 W/m・K. The 7Li(p,n)7Be reaction requires addressing lithium target cooling issues, residual 7Be nuclei (half-life 53 days), and lithium target radiation damage. In contrast, using the 9Be(d,n)10B reaction, beryllium' s high melting point and thermal conductivity enable effective water cooling to remove heat, and the residual 10B nucleus is a stable isotope without residual radioactivity or radiation hazards. Therefore, beryllium is considered as an alternative to lithium for compact neutron source target materials.

Previous BSA designs primarily include single-material moderators, multi-material moderators, liquid scatterers, and combined moderator-collimator designs. Single-material moderator designs offer simplicity in design and manufacturing and effectively reduce high-energy neutron populations, but optimizing the neutron energy spectrum is difficult with only one material, limiting therapeutic efficacy. Multi-material moderator designs combine different materials to better tune the neutron energy spectrum and improve treatment selectivity and effectiveness. Liquid scatterer designs leverage fluidity and adjustability to dynamically change neutron beam energy spectra and distributions for different treatment needs, though stability and control are challenging with risks of leakage and environmental contamination. Combined moderator-collimator designs enable precise control of neutron beam shape and direction, improving irradiation precision for tumor regions while reducing damage to surrounding normal tissue.

This paper considers using beryllium as an alternative to lithium for compact neutron source target materials, analyzes neutron yield and energy spectra from low-energy deuterium beams bombarding beryllium targets, and presents a feasible BSA design scheme for AB-BNCT devices based on the 9Be(d,n)10B reaction using a combined moderator-collimator approach.

2. Neutron Source Generation

In the late 20th century, researchers proposed the 9Be(d,n)10B neutron source for generating therapeutic neutron beams in AB-BNCT [?]. The reaction equation is:

The Q-value is 4.36 MeV. At lower deuterium beam energies, this reaction still yields relatively high neutron production with neutron energies lower than other sources ($ $6 MeV). A 1.45 MeV deuterium beam bombarding a 9 m thin beryllium target loses approximately 504 keV of energy in the target [?]. Due to the Q-value of 4.36 MeV, the 6th energy level of the residual 10B nucleus (Table 1) is preferentially populated over other states at bombardment energies around 1 MeV. Most of the reaction energy is consumed in exciting 10B, leaving only a few hundred keV as kinetic energy for emitted neutrons, resulting in very low neutron emission energies [?]. Compared to thick targets, using a thin target suppresses all reactions below the effective threshold, eliminating most high-energy neutrons while maintaining low-energy neutron yield, thereby softening the neutron spectrum and reducing subsequent moderation difficulty.

GEANT4 (GEometry ANd Tracking), developed by CERN in 1994, is a C++-based Monte Carlo simulation tool for particle transport in materials, covering various microscopic particles (electrons, neutrons, protons, X-rays, heavy ions, and radiation particles from decaying nuclides) and primarily used in nuclear physics, accelerator physics, and nuclear medicine. This study uses GEANT4' s relevant physical models to simulate the D-Be reaction.

FLUKA (FLUktuierende KAskade) is a general-purpose Monte Carlo particle transport tool capable of simulating approximately 60 different particles, including photons and electrons from 1 keV to several thousand TeV, muons of any energy, hadrons up to 20 TeV and their antiparticles, neutrons from thermal energies upward, and heavy ions. Applications include dosimetry, detector design, cosmic rays, and radiotherapy. This study uses FLUKA for the design and optimization of the entire Beam Shaping Assembly (BSA).

In the beryllium target, deuterium beams primarily undergo four reaction mechanisms: compound nuclear reactions, deuteron stripping reactions, breakup reactions, and knockout reactions [?]. The beryllium target thickness in this simulation is 9 m. Due to the thin target, no comprehensive evaluated nuclear data library currently exists for this reaction, requiring calculation of neutron yield using GEANT4' s physical models. Reference data from M.E. Capoulat et al. [?] reports a neutron yield of 1.62$\times 10^{11} n \cdot mC^{-1}.Thisstudyinvestigatedtheinfluenceofsupportmaterialsandcoolingbodiesontheneutronsourceenergysp$ $seeoriginalpaper].Thepurplecurveinthefigureshowstheneutronspectrumfrom1.45MeVdeuteriumbeambomb$ n · mC^{-1}. The results show overall agreement with reference data.

As indicated by the blue curve in [Figure 1: see original paper], neutrons above 1 MeV show minimal reduction after passing through support and cooling bodies, while neutrons below 1 MeV are significantly affected. Neutrons around 0.5 MeV are substantially reduced, and thermal neutron flux increases dramatically due to moderation by tungsten-copper (water) materials, making the results more realistic. Neutron flux decreases by 14% after passing through support and cooling materials, affecting neutrons before moderation and reducing overall neutron flux.

Information on neutron momentum, position, and emission direction from this spectrum is extracted to serve as input for the source file in subsequent FLUKA Monte Carlo simulations.

3. Beam Shaping Assembly (BSA) Design

The core task in BNCT facility design involves designing and optimizing the BSA to moderate fast neutrons to a fixed energy range of epithermal neutrons suitable for therapy. In BSA optimization, each component should be optimized based on the neutron output from upstream components. The neutron beam parameters at the BSA outlet after moderation should meet the recommended values from the International Atomic Energy Agency (IAEA) [?], as shown in .

3.1 BSA Structure

A baseline BSA model is established with an overall cylindrical structure, as shown in [Figure 2: see original paper], consisting from left to right of: reflector layer, deuterium beam channel, target, support layer, cooling body, moderating layer, collimator, and thermal neutron absorption layer. The deuterium beam is injected from the left, with beryllium target material deposited on a relatively thin layer (supported by materials such as vanadium or niobium) to avoid hydrogen embrittlement. This study does not consider these backing materials as they have minimal impact on simulation results. The target is prepared by evaporating 9 m thick Be onto a tungsten substrate. Research by L. Gagetti et al. [?] provides details on target preparation and characterization. Tungsten serves not only as a support material but also stops deuterium beams passing through the beryllium layer. Behind the beryllium-tungsten target is a copper cavity 1.5 cm thick containing water, where effective water cooling safely removes heat deposited by the beam [?]. The collimator exit radius is 7.5 cm, reducing neutron scattering and absorption losses, effectively enhancing treatment efficiency and economy while reducing radiation dose to surrounding tissues and improving patient safety and comfort.

Based on the specific information of the D-Be reaction neutron spectrum and the baseline model, FLUKA is used to design a feasible BSA scheme.

3.2 Moderating Layer

The primary function of the moderating layer is to convert as many fast neutrons as possible into epithermal neutrons. Moderating layer materials should have low scattering cross-sections in the epithermal neutron region, high scattering cross-sections in the fast neutron region, and minimal absorption cross-sections for epithermal neutrons [?]. This study employs a multi-layer moderating structure. Fluorine-containing materials exhibit excellent fast neutron moderation performance, so materials with heavy elements such as PbF2 are selected as the first moderating layer, while materials with lighter elements such as MgF2 serve as the second moderating layer [?].

Referencing numerous studies \cite{17-19} on moderating layer selection and simulation, the total length of the moderating layer combination is set to 50 cm. The first moderating layer thickness varies from 15-45 cm in 5 cm steps, with a radius of 25 cm. Simulations of different material combinations and thicknesses yield optimal candidate combinations, with results shown in [Figure 3: see original paper], [Figure 4: see original paper], and [Figure 5: see original paper], which present neutron moderation effects under different combinations.

The fast neutron component /Φepi and gamma component /Φepi represent the ratios of absorbed dose rates for fast neutrons and gamma rays to epithermal neutron flux, respectively. Φepi/Φth is the ratio of epithermal to thermal neutron flux, Φepi/Φfast is the ratio of epithermal to fast neutron flux, Φfast/Φtotal is the ratio of fast to total neutron flux, and the flux ratio J/Φ characterizes neutron beam forwardness.

As shown in [Figure 3: see original paper] and [Figure 5: see original paper], the BiF3 and MgF2 combination yields higher Φepi/Φfast ratios and lower Φfast/Φtotal ratios compared to other combinations. When the first moderating layer thickness is 45 cm, the BiF3 and TiF3 combination achieves the maximum Φepi/Φfast ratio and minimum Φfast/Φtotal. [Figure 4: see original paper] shows that Φepi increases with BiF3 thickness. While BiF3+AlF3 and PbF2+MgF2 combinations achieve similar maximum Φepi values at fixed thicknesses, their Φfast/Φtotal ratios are larger, indicating a higher proportion of fast neutrons in the total flux. The 20 cm BiF3 and 30 cm MgF2 combination shows overall optimal values for Φepi, Φepi/Φfast, and Φfast/Φtotal. Therefore, candidate moderating layer combinations are selected as: 25 cm BiF3 + 25 cm MgF2, 20 cm BiF3 + 30 cm MgF2, 45 cm BiF3 + 5 cm TiF3, and 35 cm BiF3 + 15 cm AlF3. The neutron energy spectra after passing through these moderating layer combinations are shown in [Figure 6: see original paper].

[Figure 6: see original paper] shows that the 45 cm BiF3 and 5 cm TiF3 combination yields more concentrated neutrons in the epithermal range but lower Φepi values. Due to insufficient Φepi at the output, this candidate is not considered. The 35 cm BiF3 and 15 cm AlF3 combination shows higher Φepi but also higher Φfast, making subsequent moderation more difficult. The 20 cm BiF3 and 30 cm MgF2 combination provides moderate values for Φepi, Φepi/Φfast, and Φfast/Φtotal. Therefore, the 20 cm BiF3 and 30 cm MgF2 combination is selected as the moderating layer. The 25 cm BiF3 and 25 cm MgF2 combination shows higher thermal neutron flux, which is undesirable as the BSA design goal includes minimal thermal neutron flux at the outlet. Consequently, the 45 cm BiF3 and 5 cm TiF3 combination is adopted as the moderating layer.

3.3 Reflector Layer

The reflector layer' s primary function is to reduce neutron leakage and maximize neutron flux at the BSA outlet. The reflector is cylindrical, enclosing the neutron source and moderator, and uses lead and bismuth materials that have high elastic scattering cross-sections and low absorption cross-sections in the epithermal neutron region while also serving as gamma shielding. Simulations were performed for different thicknesses of lead and bismuth reflectors, with results shown in [Figure 7: see original paper] and [Figure 8: see original paper].

[Figure 7: see original paper] and [Figure 8: see original paper] show that increasing reflector thickness significantly improves both the Φepi/Φfast ratio and Φepi, with lead outperforming bismuth. At approximately 5 cm thickness, the Φepi/Φfast ratio changes little with increasing thickness, and Φepi growth slows. At thicknesses greater than 30 cm, the Φepi/Φfast ratio shows a downward trend, and Φepi growth rate is only about 1.2%. Since this study focuses on a compact fast neutron source suitable for hospital installation, reflector thickness should be selected to minimize overall device size. Therefore, a 30 cm thick lead reflector is selected.

3.4 Supplementary Moderating Layer and Collimator

Neutrons passing through the moderating layer combination are not fully moderated to the required epithermal energy range and require further moderation through a supplementary layer. Four materials containing lighter elements—Al_2O_3, AlF_3, MgO, and MgF_2—were simulated for different thicknesses. The supplementary moderating layer is a cylindrical structure located downstream of the moderating layer combination, with the same radius as the moderating layer. Thickness varies from 5-23 cm in 3 cm steps, with results shown in [Figure 9: see original paper] and [Figure 10: see original paper].

[Figure 9: see original paper] shows that the Φepi/Φfast ratio increases with thickness for all four supplementary moderating materials, exceeding 20 at approximately 14 cm thickness. [Figure 10: see original paper] shows that epithermal neutron flux Φepi decreases with increasing thickness. For MgF_2 at 16 cm thickness and AlF_3 at 19 cm thickness, the Φepi/Φfast ratio meets requirements, with MgF_2 providing larger Φepi values. Although MgO achieves the required Φepi/Φfast ratio at lower thicknesses, its Φepi values remain lower than those of AlF_3. According to BSA design requirements, the supplementary moderating material with higher epithermal neutron flux should be selected while meeting Φepi/Φfast requirements. MgF_2 is selected with a thickness of 16 cm.

Since neutrons at the BSA outlet are relatively divergent, the collimator typically uses a conical channel structure to direct the neutron beam to the patient' s tumor site. Substituting the 16 cm MgF_2 into the conical collimator structure with an inner radius of 25 cm and outer radius of 7.5 cm yields a Φepi/Φfast ratio of 28.53. As [Figure 10: see original paper] indicates, smaller supplementary moderating layer thickness can increase epithermal neutron flux. Therefore, MgF2 is selected with a thickness of 9 cm, yielding a Φepi/Φfast ratio of 22.08 that meets requirements.

3.5 Thermal Neutron Absorption Layer

After the moderating layer combination and supplementary moderating layer, thermal neutrons are inevitably produced, with Φepi/Φth ratios of 9.19-2.55, failing to meet the IAEA minimum requirement of 20. Thermal neutrons can damage human skin and superficial tissues, necessitating a thermal neutron absorption layer before epithermal neutron beam irradiation to reduce the thermal neutron proportion. This material should have large absorption cross-sections for thermal neutrons with energies below 0.5 eV and low cross-sections in the intermediate and high-energy regions.

Common thermal neutron absorption materials are 6Li and 113Cd. 6Li has a neutron absorption cross-section of 940 b, and the 6Li(n,α) reaction produces minimal gamma contamination. 113Cd has a neutron absorption cross-section of 2100 b, with average thermal neutron absorption cross-sections of 8 b in the intermediate energy region and 0.05 b in the high-energy region, and a natural abundance of 12.2%.

Simulations were performed for LiF and natural cadmium at different thicknesses. The thermal neutron absorption layer is a thin disc structure adjacent to the supplementary moderating layer, with thickness varying from 0.01-0.08 cm in 0.01 cm steps, with results shown in [Figure 11: see original paper].

[Figure 11: see original paper] shows that the Φepi/Φth ratio for LiF increases slowly with thickness, reaching 20.4 at 0.07 cm thickness. For Cd, the Φepi/Φth ratio increases dramatically with thickness, from 39.03 at 0.01-0.02 cm thickness to 610.9 at 0.08 cm thickness—an increase of approximately 1482%—demonstrating highly effective thermal neutron absorption. Therefore, a 0.01-0.02 cm cadmium thermal neutron absorption layer meets requirements with a Φepi/Φth ratio of 39.03. At this configuration, the gamma component at the BSA outlet is /Φepi = 1.24\$$\times 10^{-15} Gy \cdot cm^2, andthefastneutroncomponentis/\Phi epi = 3.99\times 10^{-14} Gy \cdot cm^2, bothbelowtheIAEAmaximumlimitof 2\times$\$10^{-13} Gy · cm^2, satisfying requirements.

4. Conclusion

This study employs a deuterium beam bombarding a thin beryllium target, using neutrons from the 9Be(d,n)10B reaction as the source term with a yield of 1.82\$×\$10^{11} n · mC^{-1}. Through BSA design and optimization, two optimized design schemes are obtained:

1. **Scheme 1:** 20 cm thick BiF3 and 30 cm thick MgF2 combined moderating layer, 30 cm thick Pb reflector layer, 9 cm thick MgF2 supplementary moderating layer, and 0.2 mm thick Cd thermal neutron ab-

sorption layer. Air-side outlet parameters: Φepi = 1.3\$$\times 10^8 n \cdot cm^{-2} \cdot s^{-1}, \Phi epi/\Phi th = 31.52, \Phi epi/\Phi fast = 21.35, /\Phi epi = 1.35\times 10^{-13} Gy \cdot cm^2, /\Phi epi = 2.71\times$\$10^{-16} Gy • cm^2, J/Φ   0.6.

2. **Scheme 2:** 45 cm thick BiF3 and 5 cm thick TiF3 combined moderating layer, 12 cm thick Pb reflector layer, 11 cm thick Al2O3 supplementary moderating layer, and 0.1 mm thick Cd thermal neutron absorption layer. Air-side outlet parameters: Φepi = 1.05\$$\times 10^8 n \cdot cm^{-2} \cdot s^{-1}, \Phi epi/\Phi th = 39.03, \Phi epi/\Phi fast = 21.82, /\Phi epi = 1.24\times 10^{-15} Gy \cdot cm^2, /\Phi epi = 3.99\times$\$10^{-14} Gy • cm^2, J/Φ   0.6.

The epithermal neutron beam energy spectrum after moderation by these designs is shown in [Figure 12: see original paper]. A comparison of the final BSA outlet neutron beam parameters with IAEA recommended values and other worldwide epithermal neutron BSA designs is presented in . With gamma component, fast neutron component, Φepi/Φth, and Φepi/Φfast meeting IAEA recommended limits, the epithermal neutron flux requirement Φepi > 1\$×\$10^9 n • cm$^{\text{\{-2\}} \cdot \text{s}}$\{-1\} can be achieved when the beam current exceeds 0.23 A. This study provides data reference for neutron moderation and shaping in D-Be neutron sources and supports further optimization research.

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