DESIGN OF BEAM SHAPING ASSEMBLY (BSA) OF D-D NEUTRON SOURCE FOR BORON NEUTRON CAPTURE THERAPY (BNCT)

BY

MUHARANI ASNAL

A THESIS SUBMITTED IN PARTIAL FULFILLMENT OF THE REQUIREMENTS FOR THE DEGREE OF MASTER OF SCIENCE (ENGINEERING AND TECHNOLOGY) SIRINDHORN INTERNATIONAL INSTITUTE OF TECHNOLOGY THAMMASAT UNIVERSITY ACADEMIC YEAR 2016

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A Thesis Presented

By

MUHARANI ASNAL

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Abstract

DESIGN OF BEAM SHAPING ASSEMBLY (BSA) OF D-D NEUTRON SOURCE FOR BORON NEUTRON CAPTURE THERAPY (BNCT)

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Boron Neutron Capture Therapy (BNCT) has for many decades been promoted as an innovative form of radiotherapy and has the potential to be the ideal form of treatment for many types of cancers. To properly utilize BNCT method, neutrons must have a specific properties, where can be achieved by treating with a particular system, called a beam shaping assembly (BSA). By using appropriate geometry configuration and material selection for BSA, the high quality of neutron beam can be achieved. In this thesis, a BSA for modifying fast neutrons from D-D nuclear reactions for BNCT was designed using the Monte Carlo simulation code Particle Heavy and Ion Transport code System (PHITS). The proposed BSA consisted of 4 cm of Pb as a multiplier, 16 cm of TiF_3 as a first moderator, 60 cm of AlF_3 as a second moderator, 30 cm of Al_2O_3 as a reflector, and 3 cm of Li as a thermal filter. These results are evaluated with the standard recommended by the International Atomic Energy Agency (IAEA). The results showed that the proposed BSA was capable of producing neutron flux with $\varphi_{epi}/\varphi_{fast}$ of 27 and $\varphi_{epi}/\varphi_{thermal}$ of 126, satisfying the IAEA recommendation of neutron beams used for BNCT. It was also found that the proposed BSA showed a better performance compared to the existing BSA designs in terms of the epithermal neutron output quality without the need of fast neutron filters.

Keywords: BNCT, BSA, D-D reaction, Monte Carlo simulation, epithermal neutron, moderator.

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Chapter 1
Introduction

1.1 Overview

1.1.1. Cancer and human health

Cancer is a group of abnormal cells that can uncontrollably increase their and can invade other tissues. Glioblastoma (GBM) is a form of brain tumor and is characterized by its rapid growth in the surrounding healthy tissue. It arises from astrocytes, a supportive tissue of the brain (Parsons et al., 2008). GBM is extremely malignant or cancerous. This is because the cells are supported by large network of blood vessels and therefore are able to reproduce very quickly (Stupp et al., 2005). The clinical history of a patient with GBM is typically short of less than 3 months in more than 50% of patients. Common presenting symptoms are neurologic deficit such as motor weakness, headache and increased intracranial pressure. Treatment for preventing GBM is currently unavailable and there is no clear way to prevent it. The commonly used methods for GBM therapy include surgery, chemotherapy, and radiotherapy. GBM cannot be cured surgically and thus surgery merely attempts to establish a pathologic diagnosis and to relieve any mass effect (Roa et al., 2004). The addition of radiotherapy to surgery can increase the survival rate of patience (Daumas-Duport et al., 1988). The responsiveness of GBM to radiotherapy also varies. Chemotherapeutic agents, targeted molecular agents, and antiangiogenic agents may increase the therapeutic effect of radiotherapy (Mukundan et al., 2008).

In fact, such cancer treatments are proven ineffective. Therefore, developing more appropriate techniques for this cancer is important and technological interesting. The prerequisite for an ideal cancer therapy is capability of the proposed technique to selectively destroy tumor cells without resulting in any damages to surrounding normal cells. One of the promising methods for the GBM brain tumor is boron neutron capture therapy (BNCT).

1.1.2. Boron Neutron Capture Therapy (BNCT)

BNCT is primarily targeted at tumors which are difficult to treat with conventional therapy, such as GBM. BNCT was proposed in 1936 by Locher, a scientist at the Franklin Institute in Pennsylvania, USA (Sweet, 1951). The first clinical trials took place at Brookhaven National Laboratory in 1951 and Massachusetts Institute of Technology in 1954 (Barth et al., 2005). Initial clinical trials were unsuccessful due to normal tissue necrosis attributed to high concentrations of boron in normal brain capillaries and the poor penetration depth of thermal neutron beams. BNCT was resumed in Japan in 1968 using more selective boron compounds (Nakagawa & Kageji, 2012). Results were encouraging although they indicated that the survival times of these patients were no better than for those receiving conventional radiotherapy.

1.1.2.1. The principles of BNCT

The rationale of using BNCT is based on the nuclear interaction of ^{10}B, which is loaded to tumor cells, with thermal neutrons (Figure 1.1). This nuclear interaction generates high linear energy transfer (LET) α and ^{7}Li particles through the boron neutron capture reaction, ^{10}B (n, α) ^{7}Li (Eq. 1.1) (Yamamoto et al., 2013). The energy of such heavy particles (2.34 MeV) can be locally deposited in the range of 5–9 µm, which corresponds to the diameter of tumor cells. Therefore, high-LET irradiation of tumor cells without unwanted damage to normal cells is expected.

$$^{10}B + n \rightarrow [11B]^{*} \rightarrow \alpha + 7Li + 2.34\ MeV \qquad (1.1)$$

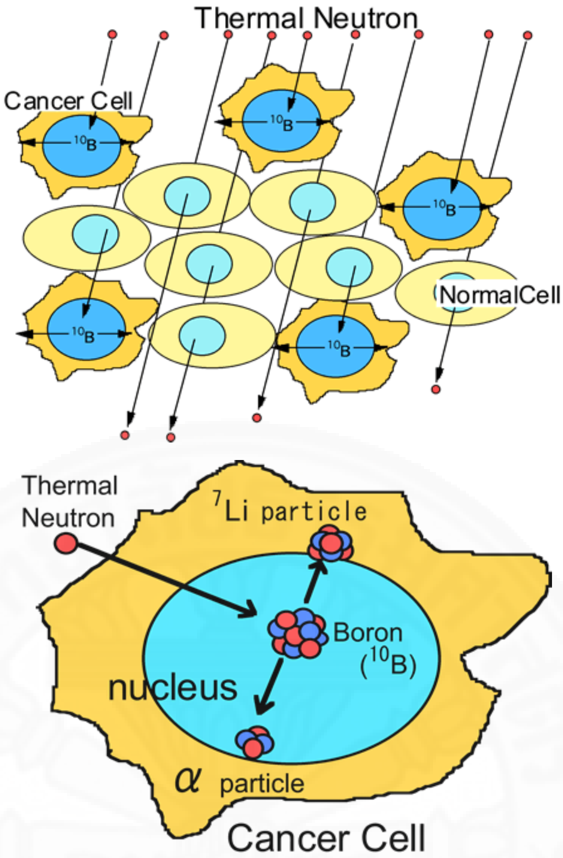


Figure 1. 1 Schematic illustration of neutron captures reaction in BNCT (Miyatake et al., 2009). As seen, the cancer cells are selectively destroyed without damage for adjacent normal cells.

Taking all of the above-mentioned features of BNCT into account, the critical factors for successful therapy would be matching the neutron source with ^{10}B-containing agent, the amount of LET particles, and the selectivity of the ^{10}B-containing agent in tumor cells. Due to the fact that the location of GBM is typically near the brain center surrounded by healthy tissues, tumor cells cannot be destroyed by thermal neutrons. This is because the thermal neutrons penetrate weakly and thus can stop in the skin or in other healthy tissues. The suitable neutrons for GBM therapy are those having the energy in epithermal range of 1 eV–10 keV (Cerullo et al., 2004).

1.1.2.2. Neutron sources for BNCT

There are three basics sources of neutron beam: nuclear reactors, radioisotope sources and particle accelerators (Barth et al., 1999). Nuclear reactors can provide high level of neutron flux. However, nuclear reactors are complex and expensive. Safety and practical features of particle accelerators triggered many researchers to employ particle accelerators in hospitals as an example, neutron generators based on D-T and D-D fusion reaction. Neutrons are emitted with energy of 2.45 MeV from D-D and 14.1 MeV from D-T reactions (Mills, 1971).

Neutrons are divided in three classes according to their energy:

- thermal (E_n < 0.5 eV)
- epithermal (0.5 eV < E_n < 10 keV)
- fast (E_n > 10 keV)

Even though thermal neutrons can efficiently interact with ^{10}B, their limited depth of penetration makes them unsuitable for destroying tumors well below the surface. Epithermal neutrons are then preferred for clinical therapy since they lose energy and become thermal as they penetrate tissues. Thermal beams remain the best solution for surface treatments such as melanoma or glioma treatments with open craniotomy. Figure 2.2 shows the trend of thermal neutron flux for thermal and epithermal beams.

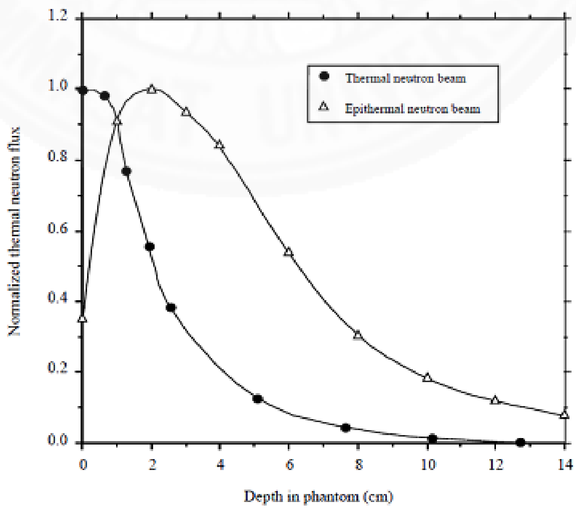


Figure 1. 2 Comparison of in-depth thermal flux distributions for thermal and epithermal neutrons (Raffaele, 2012).

General desirable beam properties can be summarized as follows:

- Minimum beam intensity of 10^9 epithermal neutrons $cm^{-2}s^{-1}$. Lower intensities often results in unacceptable longer irradiation times, while higher intensities usually mean worse beam quality.
- The fast neutron component should be kept as lower as possible.
- The thermal component results in an additional damage to the scalp; the ratio of thermal flux to epithermal flux should be around 0.05.

1.1.2.3. Boron compounds

In BNCT, dose targeting is achieved by selectively loading the stable isotope ^{10}B into the malignant tissue via a tumor-selective boronated pharmaceutical infused directly into the patient's bloodstream. The biochemical selectively of the boronated compound allows large concentrations of ^{10}B to accumulate in the tumor cells relative to normal tissue (3 to 4 times more), essentially differentiating normal and cancer cells. The ^{10}B compound alone is normally not toxic to cells. It is eliminated from the body within a reasonable time frame after infusion.

1.1.2.4. Beam Shaping Assembly (BSA)

To ensure the applicability of neutrons generated by compact neuron sources, i.e. a compact neutron sources based on D–D nuclear fusion reactions, a Beam Shaping Assembly (BSA) must be required. This is because the radiation field produced by compact neuron sources consists of some radiation dose components, namely fast and thermal neutron doses and gamma dose. The clinical neutron beams produced from BSA is allowed to include only minimal contaminants from the above-mentioned dose components such that the background dose to healthy tissue is kept within the tolerance limits. So, the main functions of BSA are to moderate the fast neutrons produced by the nuclear fusion reactions to epithermal energy range and to eliminate the formation of thermal neutrons (Rahmani & Shahriari, 2011). The main characteristic of materials suitable for BSA is its effectiveness in reducing fast neutron flux while enhancing epithermal flux. These kinds of materials thus allow for efficient slowing down from the fast to the epithermal energies without removing these epithermal neutrons. The net result would be an accumulation of epithermal neutrons. Many studies have searched for optimal materials for accelerator-based BNCT. Several materials which are proven to be good for BSA are Fluental and Aluminum and Fluorin compounds. Fluental is a composite material consisting of a mixture of AlF_3 (69%), Al (30%), and LiF (1%). In fact, the most common moderator materials in BSA for BNCT are Al and AlF_3. They are used mainly due to their low cost compared to Fluental. However, their low density compared to Fluental is one of their main drawbacks. Overall, BSA is designed with appropriate choice of geometry and materials to achieve sufficient beam intensity and suitable beam parameters.

1.2. Motivation

The geometry and materials used in each BSA design play a crucial role in determining the characteristics of the resulting neutron beam. Therefore, it is needed to carefully design the BSA so that the resulting neutron beam from compact neutron reactors can be effectively applied for BNCT. Studies have been carried out to investigate the suitability of BSA designs with compact D-D neutron sources for BNCT (Durisi et al., 2007; Eskandari & Kashian, 2009; Fantidis et al., 2013; Rasouli & Masoudi, 2012; Rasouli et al., 2012). The MCNP4B Monte Carlo code is usually used for designing BSA. To give an instance, a BSA with a compact D–D neutron generator was simulated using the MCNP4B Monte Carlo code (Fantidis et al., 2013). The optimum moderator design is a conic part made of D_2O followed by a TiF_3 layer. An epithermal neutron beam with appropriate quality can be achieved by using BiF_3 as spectrum shifter and γ rays filter, Ti as fast neutron filter, and Li as thermal neutron filter. Unfortunately, the obtained epithermal neutron flux (1.17×10^6 n/cm^2 s) cannot satisfy the IAEA recommended values for clinical treatment.

Although the output neutron beam characteristics of existing BSA designs in term of $\varphi_{epi}/\varphi_{fast}$ and $\varphi_{epi}/\varphi_{thermal}$ satisfy the IAEA criteria, their values are still relatively low. Therefore, in this research, a beam shaping assembly with D-D and D-T compact neutron generators is designed not only to fulfill the IAEA criteria but also to feature appreciable values of $\varphi_{epi}/\varphi_{fast}$ and $\varphi_{epi}/\varphi_{thermal}$.

1.3. Aims of the study

- To design a beam shaping assembly (BSA) which is capable of producing an epithermal neutron beam for BNCT based on neutrons from D-D reactions.
- To compare the performance of the proposed BSA with some existing BSA designs, i.e. by Eskandari and Kashian (Eskandari & Kashian, 2009), Rasouli et al. (Rasouli et al., 2012), and Rasouli and Masoudi (Rasouli & Masoudi, 2012) in term of the output neutron beam characteristics

1.4. Scope of the study

- The neutron sources and BSA configuration are modeled with the particle heavy and ion transport code (PHITS).
- The simulated D-D neutron generators are assumed to produce fast neutrons with the energy of 2.45 MeV.
- The input fast neutron beam is assumed to possess a diameter of 1.7 cm with a neutron flux of 10^{13} and 10^{15} n/s for D-D and D-T neutron generators, respectively (Leung, 2009).
- Optimum condition for producing epithermal neutrons is used together with the IAEA standard of neutron beams for BNCT.

Chapter 2
Literature Review

2.1 Clinical trials of BNCT for tumors

The first BNCT trials were performed in the USA around 1960. Promising results in the treatment of various cancers, especially head and neck cancer and recurrent glioma, have been documented. The two boron compounds currently used in BNCT are isodium mercaptoundecahydro-closo-dodecaborate (BSH) and boronophenylalanine (BPA). BNCT is still being used in clinical trials and have demonstrated some very good results.

Moreover, the development of linear accelerators specifically for BNCT applications has also been progressed. All these facts lead to optimism to the future of BNCT. Japan has the most pioneering treatment of patients with BNCT, while the patient irradiations were mostly done in Finland. As an example, a 62-year-old man patient with recurrent lung cancer in the previously irradiated chest wall was treated with two-fractionated BNCT (Suzuki et al., 2012). BPA was used as a boron compound in clinical trials of BNCT. Before irradiation, BPA was administered intravenously at a rate of 200 mg/kg/h for 2.0 h in a BPA-fructose (BPA-f) solution. During neutron irradiation, administration of BPA was continued at a rate of 100 mg/kg/h. The neutron beam for BNCT were produced from the Kyoto University Reactor (KUR). Treatment planning and analysis of dose distributions is carried out using the SERA system. At 51 and 52 months after initial radiotherapy, the two fractions of BNCT were delivered with a one-month interval between them. In each of the two BNCT sessions, irradiation was performed with epithermal neutron beams with a 15 cm circular collimator and the same beam axis. Results showed that most of the tumor regressed at seven months after the BNCT. No acute or late adverse events were observed.

2.2 BSA design to generate epithermal neutron based on D-T neutron source for BNCT

2.2.1 Introduction

Boron Neutron Capture Therapy (BNCT) is an indirect radiotherapy for destruction of cancer cells. To utilize BCNT, ^{10}B enriched compounds must be first introduced into the patient's body. The tissues are then irradiated by a low-energy neutron beam, which can induce $^{10}B(n,^{4}He)^{7}Li$ reactions producing secondary charged particles with high biological effectiveness.

One of the critical parameters in BNCT is the neutron flux of a neutron source, which must be in an appropriate rate for a sufficiently long enough time. The neutron source providing the required neutron beam with high neutron flux has previously seen only in a nuclear reactor. However, a suitable nuclear reactor for such purpose is expensive and difficult to be realized in or near urban areas. This leads to the development of other neutron sources for BNCT. For example, a compact neutron generator based on the D-T fusion reaction was proposed as a suitable neutron source for in-hospital treatments (Rasouli et al., 2012). It has greater safety, lower energy for an incident deuteron beam, lower cost, smaller size, and higher social acceptability.

Owing to the fact that the typical neutron energy emitted from D-T fusion reaction is 14.1 MeV, these neutrons cannot be used directly in BNCT. Therefore, they are moderated to the epithermal energy range, between 1 eV and 10 keV. For this purpose, neutrons must be treated within a particular system, called a beam shaping assembly (BSA). By using appropriate geometry configuration and material selection in BSA design, the quality and intensity of neutron beam can be optimized. Further, as the intensity of the beam determines the treatment time, it must be considered in the BSA design as well. According to the International Atomic Energy Agency (IAEA) recommendation, epithermal neutron flux should be on the order of 10^9 n/cm^2 s. It is pivotal to note that since the neutron flux usually decreases greatly when neutrons pass through different components of BSA (Rasouli et al., 2012), it is necessary to increase the number of neutrons emitted from the neutron source. In this paper, the main components of BSA are compared and three BSA designs are discussed.

2.2.2 BSA Components

As mentioned earlier, a BSA is basically designed to moderate high energy neutrons to lower energies. In addition, it must remove fast and thermal neutrons and gamma contaminations. A BSA consists of the multiplier, moderator, neutron filter, reflector, gamma shielding and collimator as major components. In order to obtain a suitable neutron beam for BNCT, a proper design must be employed.

2.2.2.1 Multiplier

A multiplier is used to increase the number of neutrons emitted from a neutron source, due to the fact that the neutron flux is significantly decreased when neutrons pass through different materials of the BSA. Hence, the material of the multiplier should be properly chosen. Uranium is a typical material used as a neutron multiplier to increase the number of neutrons via fission reactions.

Rasouli et al. used an isotropic source of 14.1 MeV neutrons placed at the centre of a sphere made of natural uranium to determine the optimal thickness of uranium, generating the highest flux of neutrons (Rasouli et al., 2012). The number of neutrons per neutron source was found to increase with the uranium's thickness and reached a maximum value with a 14 cm radius. They also compared the geometry of uranium, namely cylindrical and spherical. It was found that the uranium geometry played a minor role on neutron multiplication. Two cylinders containing uranium at the maximum point generate approximately the same number of neutrons as generated by the spherical uranium. Thus, a sphere is certainly preferable due to its lightness.

Eskandari and Kashian, employed Pb and ^{238}U as multiplier materials. The large cross section of Pb for (n, 2n) reaction compensate for the neutron losses by leakage and absorption during moderation (Eskandari & Kashian, 2009). Moreover, the neutron flux was maximized by the use of ^{238}U as a neutron multiplier. In this design, Pb was modelled with 1, 2, 3, 4, 5, 6, 8, 10, and 12 cm thicknesses. The suitable thickness for Pb was found to be 3 cm. Further, the layer with ^{238}U was modelled with 0.5, 1, 1.5, 2, 2.5, 4, and 5 cm thicknesses, and the suitable thickness was found to be 2 cm.

Bi, U, and Pb containing acceptable (n, 2n) cross sections for 14 MeV neutrons were examined using MCNP5 code (Eskandari & Kashian, 2009). Results showed that 5 cm Bi was considered as a suitable multiplier. Pb was also another good choice of a multiplier. However, due to gamma emissions, U was not recommended as a multiplier.

2.2.2.2 Moderator

For the moderator, Fluental and Fe are considered to be suitable materials (Koivunoro et al., 2003). Fluental is a neutron moderator material developed at VTT in Finland and composed of 69% AlF_3, 30% Al and 1% LiF. Fe is however preferred due to its lower cost and higher abundance. Magnesium fluorine (MgF_2) is also proven useful for producing neutrons in the epithermal energy range [8]. Although U is still used as a moderator as well, it was recently considered an improper material owing to its harmful gamma emissions (Eskandari & Kashian, 2009).

Verbeke et al. proposed medium materials such as Fluental, Fe, Al, Ni, AlF_3, Al+AlF_3, and LiF as moderators for BNCT (Verbeke et al., 2000). These materials were proven to approximately fulfil IAEA criteria. In fact, because of their low cost compared to Fluental, Al and AlF_3 are commonly used as moderator materials in BSA for BNCT. However, the low density of Al and AlF_3 compared to Fluental is one of their main drawbacks. Relatively thick Al and AlF_3 are required for the same neutron attenuation as achieved with Fluental.

De Boer evaluated Al followed by Al_2O_3 or AlF_3 near the beam exit as a moderator (de Boer, 2008). These combinations exhibited efficient performance since the O and F cross sections fill in the valleys between the energy resonances peaks of Al. Results also showed that AlF_3 was a suitable moderator for neutrons with energies less than 10 keV, whereas Al_2O_3 was a better moderator for fast neutrons with energies which are higher than 10 keV.

Miyamaru and Murata evaluated D_2O, Fluental, carbon, and beryllium as moderator materials (Miyamaru & Murata, 2011). Results showed that D_2O was suitable for epithermal neutron production with the highest flux and most decreased number of fast neutrons. D_2O, H_2O, Li/D_2O, and Fe were also evaluated as moderator materials and D_2O was found to be a suitable material in terms of both absolute and relative thermal-epithermal fluency in the emergent neutron beam.

For finding proper moderators, Rasouli et al. investigated 16 different materials, namely TiF_3, Fluental, AlF_3, Al_2O_3, MgF_2, BeO, Fe, Al, H_2O, CF_2, Mn, PbF_2, LiF, Co, Cu and PbF_4 (Rasouli et al., 2012). In their work, the geometry of the moderator and reflector are cylindrical. The epithermal flux and the ratio of epithermal neutron flux over fast neutron flux ($\varphi_{epi}/\varphi_{Fast}$) associated with these materials were calculated using the MCNP4C code (Rasouli et al., 2012). Results showed that TiF_3 with 23 cm thickness was suitable material for a moderator. However, although the epithermal flux for TiF_3 reached its maximum value, the resulting $\varphi_{epi}/\varphi_{Fast}$ did not satisfy the IAEA's recommended value, which might be due to the use of uranium as a multiplier that can intensify the fast neutron flux. For increasing $\varphi_{epi}/\varphi_{Fast}$, a second moderator was used to reduce the number of fast neutrons. When 23 cm thick TiF_3 was selected as the first moderator, the value of $\varphi_{epi}/\varphi_{Fast}$ of 40 cm Fluental as the second moderator was shown to be larger than the critical value recommended by IAEA. Thus, it is suitable to use Fluental as the second moderator in this case.

It is known that materials containing F or Mg have a maximum value of fast to epithermal over macroscopic absorption cross sections ($\sum s_{f/epi}/\sum_{\gamma}$) (Eskandari & Kashian, 2009). In terms of neutron accumulation in epithermal energy range during the slowing down from source energies, these materials are claimed to be better than other moderator materials. Due to this reason, Eskandari and Kashian also used AlF_3 as a moderator. It has a large ratio of $\sum s_{f/epi}/\sum_{\gamma}$. Based on their work, the ratio of fast neutrons to total neutron flux between 60 and 70 cm of AlF_3 was constant and therefore 60 cm AlF_3 was selected as a moderator (Eskandari & Kashian, 2009).

Due to the fact that a good moderator for BNCT should not induce high gamma ray contamination, a material inducing less gamma dose rate must be selected as a moderator material. Based on these criteria, Fe was selected with 50 cm length and 80 cm thickness as the moderator material (Eskandari & Kashian, 2009).

Furthermore, in order to reduce cost, successive stacks of Al, polytetrafluoroethylene (PTFE) and LiF (Al/PTFE/LiF) were used as a moderator (Burlon et al., 2004). The reason is that the neutron interaction cross section in Al and PTFE can effectively moderate fast neutrons. Results showed an acceptable behaviour of the proposed moderator and the advantage of irradiating the target with near-resonance-energy protons (2.3 MeV) because of the high-neutron yield at this energy. This leads to production of less fast neutrons and ultimately the lowest treatment times. The 34 cm Al/PTFE/LiF moderator was found to be the suitable option.

2.2.2.3 Fast and thermal neutron filter

One of the key considerations in designing a BNCT beam is reducing the fast neutron component of the incident beam. In many cases, the fast neutron flux cannot be properly decreased by the moderator due to a surplus of the fast and thermal neutrons. Because of this, a fast neutron filter material that can reduce the fast component of the flux, resulting in an increased epithermal one, is required. The material commonly used is Al or its compounds (Burlon et al., 2004). According to the recommendations of IAEA, the desirable minimum beam intensity would be 10^9 epithermal neutrons $cm^{-2}s^{-1}$. Elements with good thermal neutron absorbers are ^3He, ^{10}B, ^6Li, ^{14}N, and Cl. Since ^3He is very rare and has a high potential as an energy source, it is not very useful as a thermal neutron absorber [9].

^6Li was considered a suitable thermal neutron filter due to smaller the release of gamma rays in the process. Its high thermal absorption cross section helps to remove thermal neutrons from clinical neutron beams. Thus, lower thermal contamination and lower gamma contamination due to thermal neutron absorption is the result. Gao used ^6Li as a filter for BNCT(Gao, 2005). The filter was able to increase the average energy of the epithermal neutrons in the epithermal neutron beam. Venhuizen [17] also examined the performance of gadolinium (Gd) as the thermal neutron filter using MCNP calculations. Results, however, showed that Gd is not suitable for this application owing to gamma contamination issue.

Because of its high inelastic scattering cross section, Fe was used as neutron filter material (Kiger III et al., 1999). It decreased the fast neutron flux with energy up to 14.1 MeV. Fe with a thickness of 4 cm was found to satisfy the IAEA's criteria because D_{fn}/φ_{epi} was less than 2×10^{-13} Gy cm^2. Further, due to filter addition, the fast and thermal neutron contaminations was capable of being removed even though epithermal flux is unavoidably reduced.

Faghihi also studied many materials as the filter and recommended Al(40%) + AlF_3(60%) as the suggested filter since it has low epithermal neutron absorption cross sections, high thermal absorption cross section and smaller radiation capture cross section.

2.2.2.4 Reflector

A reflector is used for directing the neutrons to the beam port. For finding a cheaper alternative reflector, Uhlar et al. tested a two-layer reflector; tungsten (W) as the inner part and Mo as the outer part. Approximate with the same performance, the mass of the W/Mo reflector is five times smaller than to the single component reflector made of W.

A research work by Burlon et al. confirmed that Pb is a suitable choice as reflector (Burlon et al., 2004). Pb has also shown better performance than graphite. Rasouli et al. also evaluated the possibility of using Pb and BeO as the reflector (Rasouli & Masoudi, 2012). Their different thicknesses were assessed to determine their reflective capabilities. Pb was also used as a reflector material for D–T neutrons, even though with a Bi collimator, spectra calculations gave similar results.

The use of graphite and boranyloxyboron (B_2O) reflectors were also investigated to increase both relative and absolute thermal-epithermal neutron fluency (Burlon et al., 2004). The best results in terms of thermal-epithermal fluency were obtained using a B_2O reflector. For a reflector thickness of 10 cm the relative thermal-epithermal fluency reaches a maximum value of 85%.

2.2.2.5 Collimator

A collimator is used to focus output neutron beam to the head phantom. Bi is a commonly used material for a collimator [6]. Reflector material such as Lithium Polyethylene in a trapezoidal shape is also occasionally used to collimate output neutron beam.

Uhlar et al. utilized Pb supplemented with a Ni part as a collimator (Uhlář et al., 2013). In a further study, they also employed molybdenum (Mo) supplemented with a nickel part. This is because at low neutron energies, nickel elastic cross section is higher than that of Mo and the Ni absorption cross section is lower than the Mo absorption cross section for a broad energy interval of moderated neutrons.

2.2.2.6 Gamma shielding

Gamma shielding is used to reduce gamma rays originated from the nuclear reactions and neutron capture in different BSA materials. Bi is normally used for this purpose. For instance, Rasouli et al. employed Bi for gamma shielding (Rasouli et al., 2012). Results showed that using 2.6 cm Bi, D_{γ}/φ_{epi} was able to be decreased to lower than 2×10^{-13} Gy cm^2. Thus, it is suitable for BNCT.

2.2.3 BSA Models

In this section, three BSA models for BNCT are discussed. The first one is a BSA model proposed by Rasouli and Masoudi (figure 2.1) (Rasouli & Masoudi, 2012) are used Natural uranium as a neutron multiplier and thick layers of TiF_3 and Al_2O_3 as moderators. These materials are surrounded by a thick Pb reflector. Ni and Li-Poly are used as shield and collimator, respectively. This configuration shows low contamination of the fast and thermal neutrons and gamma at the beam port, which satisfies almost all IAEA criteria.

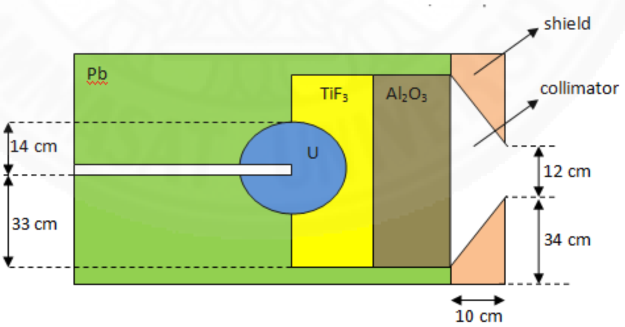


Figure 2. 1 The BSA model proposed by Rasouli and Masoudi (Rasouli & Masoudi, 2012).

Rasouli and colleagues also designed BSA for BNCT based on the use of 14 cm in radius metallic uranium as multiplier system for D–T neutron source and moderator/filter/reflector arrangement (Rasouli et al., 2012). TiF_3 with 23 cm in thickness and Fluental with 36 cm in thickness are used for the moderator to achieve a proper epithermal neutron flux. A configuration of 4 cm Fe, 1 mm Li, and 2.6 cm Bi are used for fast neutron, thermal neutron, and gamma ray filters, respectively, as illustrated in figure 2.2.

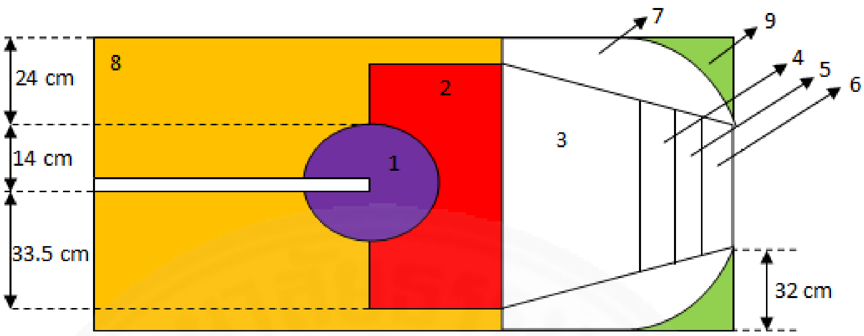


Figure 2. 2 The BSA model proposed by Rasouli et al. (Rasouli et al., 2012). Remarks: 1 is 14 cm uranium, 2 is 23 cm TiF3, 3 is 36 cm Fluental, 4 is 4 cm Fe, 5 is 1 mm Li, 6 is 2.6 cm Bi, 7 is Pb as collimator, 8 is Pb as reflector, 9 is shield.

Rahmani and Shahriari proposed a BSA model containing layers of Mg, Al, Fe, Pb, Bi, C, and Ni joined with their oxide and fluoride compounds as illustrated in figure 2.3 (Rahmani & Shahriari, 2011). In this model, 10 cm of Ni is selected as a collimator material in conical shape. Pb with 25 cm in thickness, 5% borated polyethylene, and 1 mm Cd are used as a reflector, neutron shield, and thermal neutron filter, respectively.

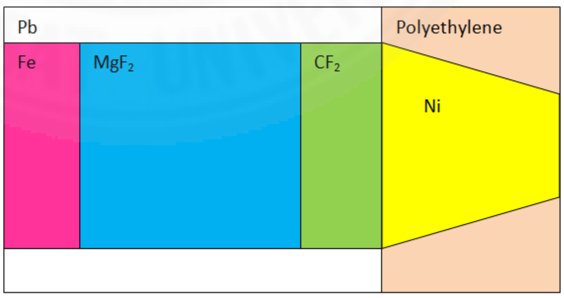


Figure 2. 3 The BSA model proposed by Rahmani and Shahriari, (Rahmani & Shahriari, 2011).

It should be noted that as the suitable option for the treatment of deep-seated tumors, the epithermal neutrons should possess a minimum intensity of 5×10^8 n/cm^2s for a reasonable time treatment. Therefore, selecting an appropriate neutron source able to provide this epithermal flux is pivotal before undertaking BSA design.

The neutron yield of the available neutron sources capable of satisfying such criteria is in the range of $6.6 \times 10^{11} – 4.4 \times 10^{14}$ n/s (Rasouli & Masoudi, 2012).

The BNCT parameters of three configurations are presented in table 2.1. Based on the BNCT free beam parameters of those three BSA configurations, it was found that only the BSA designed by Rasouli et al. satisfies all IAEA criteria (Rasouli et al., 2012). Although the BSA proposed by Rasouli and Masoudi cannot satisfy all IAEA criteria (Rasouli & Masoudi, 2012), its neutron beam is effective for deep-seated brain tumor treatments even with D–T neutron generator yielding as low as 2.4×10^{12} n/s. It was found in this configuration that with increase in the neutron source yield, the treatment time decreases. Also, a shorter treatment time can be achieved with the cost of high neutron source intensity. Thus, considering the trade-off between reduction of treatment time and neutron source intensity is vital. In those three configurations, use of specific filters is very important for removing the fast and thermal neutrons and gamma contamination from neutron beam. However, the epithermal neutron flux is decreased.

Table 2. 1 BNCT parameters of the three BSA configurations.

BSA model	$\varphi_{epi} \times 10^9$ (n/cm^2 s)	$\varphi_{epi}/\varphi_{thermal}$	$\varphi_{epi}/\varphi_{Fast}$	$D_\gamma/\varphi_{epi} \times 10^{-13}$ (Gy cm^2)	$D_{fn}/\varphi_{epi} \times 10^{-13}$ (Gy cm^2)
Rahmani and Shahriari, (Rahmani & Shahriari, 2011)	8.19	383	17.20	1.18	7.98
Rasouli et al. (Rasouli et al., 2012)	4.43	121.2	23.75	1.98	0.59
Rasouli and Masoudi (Rasouli & Masoudi, 2012)	1.04	20.21	-	5.79	0.67
IAEA criteria	>0.5	>100	>20	<2	<2

Chapter 3
Comparison of Existing Designs

3.1 Introduction

One of the critical parameters in BNCT is the neutron flux of a neutron source, which must be in an appropriate rate and energy range. The neutron source providing the required neutron beam with high neutron flux has previously seen only in a nuclear reactor. However, a suitable nuclear reactor for such purpose is expensive and difficult to be realized in or near urban areas. This leads to the development of other neutron sources for BNCT. One of them is a compact neutron generator based on the D-T fusion reaction.

Due to the fact that the typical neutron energy emitted from D-T fusion reaction is 14.1 MeV, these neutrons cannot be used directly in BNCT. Therefore, they are moderated to the epithermal energy range, between 1 eV and 10 keV. For this purpose, neutrons must be treated within a particular system, called a beam shaping assembly (BSA). By using appropriate geometry configuration and material selection in BSA design, the quality and intensity of neutron beam can be optimized. Further, as the intensity of the beam determines the treatment time, it must be considered in the BSA design as well. According to the International Atomic Energy Agency (IAEA) recommendation, epithermal neutron flux should be on the order of 10^9 n/cm^{2}s.

3.2 Descriptive Of Code

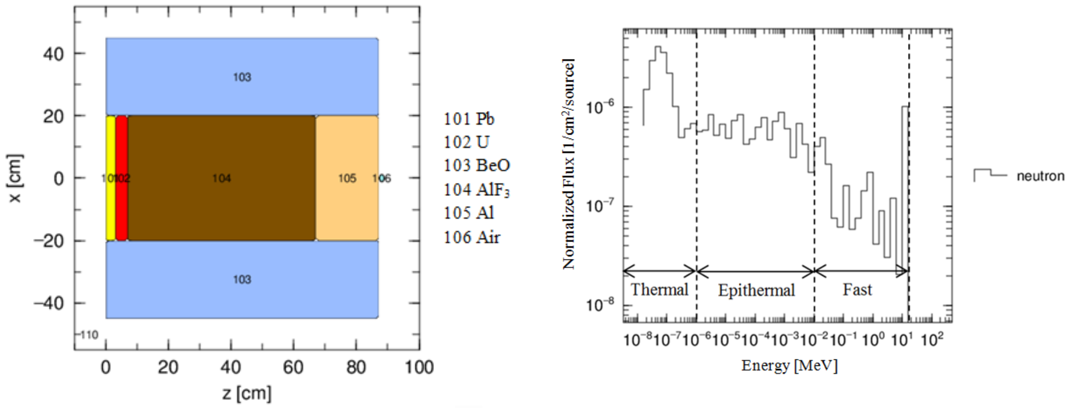
In order to produce high epithermal neutron (energy range from 1 eV to 1×10^{-2} MeV) flux from D-T neutron generators using BSA, an accurate information of the interactions between high energy neutrons and materials are necessary. Particle and Heavy Ions Transport code System (PHITS), as one of well-known Monte Carlo particle transport codes (for instance: FLUKA, PHITS, GEANT4, MARS15, MCNPX, and SHIELD), is capable of elucidating the information of the interactions between high energy neutrons and materials. PHITS can simulate behaviours of particles and heavy ions under influence of neutron flux over wide energy ranges and deals with the transport of all particles (nucleons, nuclei, mesons, photons, and electrons) over wide energy ranges, using several nuclear reaction models and nuclear data libraries (Sato et al., 2013).

The PHITS code has been used for various research fields such as radiation science, accelerator and its shielding design, space research, medical application, and material research. Niita et al. (Niita et al., 2006) study three applications of the PHITS including spallation neutron source, heavy ion therapy and space radiation. It was shown that PHITS has great ability of carrying out the radiation transport analysis of almost all particles including heavy ions within a wide energy range. However, use of PHITS code for BSA designs has not been reported. Therefore, in this study, PHITS is used to carry out a series of simulations for three BSA designs, developed for producing an epithermal neutron flux from a D-T neutron source.

The simulations using PHITS code was performed for three BSA designs proposed by Eskandari and Kashian (Eskandari & Kashian, 2009) (design A), Rasouli and Masoudi (Rasouli & Masoudi, 2012) (design B), and Rasouli et al. (Rasouli et al., 2012) (design C), to investigate their capabilities to produce epithermal neutron. The geometry of those designs has a function to draw in 2D and 3D graphical geometry plot definition. It is assumed in this work that all designs of BSA considered are a cylindrical shape. In each design, it is composed of six different layers, namely, neutron multiplier, neutron moderator, fast neutron filter, thermal neutron filter, shielding and collimator. Furthermore, it is assumed that the neutrons are emitted monoenergetically and the neutron yield of D-T generator is 1.45×10^{14} n/s.

3.2 Results and Discussion

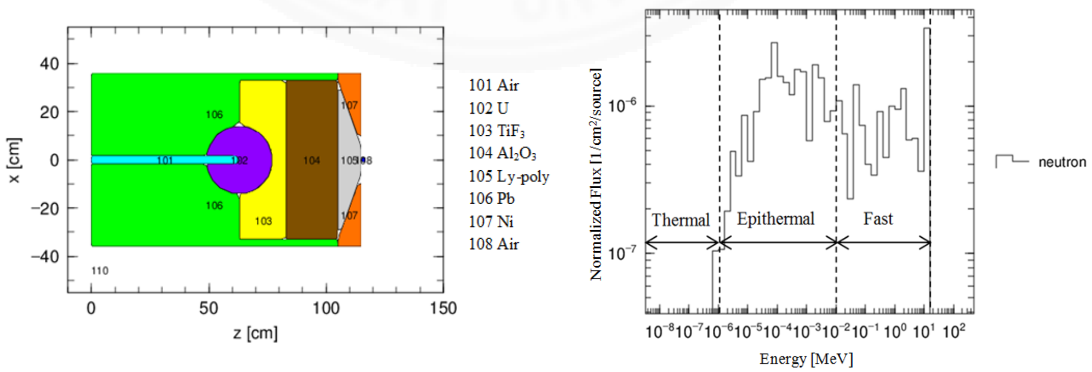
Figure 3.1 (a) shows the design A, composed of 3 cm Pb as first multiplier, 2 cm U as second multiplier, 25 cm BeO as reflector, 60 cm AlF_3 as moderator, and 20 cm Al as filter. The out coming value of epithermal neutron flux is calculated to be 1.73×10^9 n/cm^{2}s. A significant thermal neutron flux is, however, generated (258.2×10^9 n/cm^{2}s) by this simple design. Further, as can be seen from the relatively low value of fast neutron flux (0.47×10^9 n/cm^{2}s), Al seems to be a suitable material for filtering the fast neutron.



(a) **(b)**

Figure 3. 1 The BSA design (a) and neutron beam port flux per neutron source versus energy (b) proposed by Eskandari and Kashian (Eskandari & Kashian, 2009).

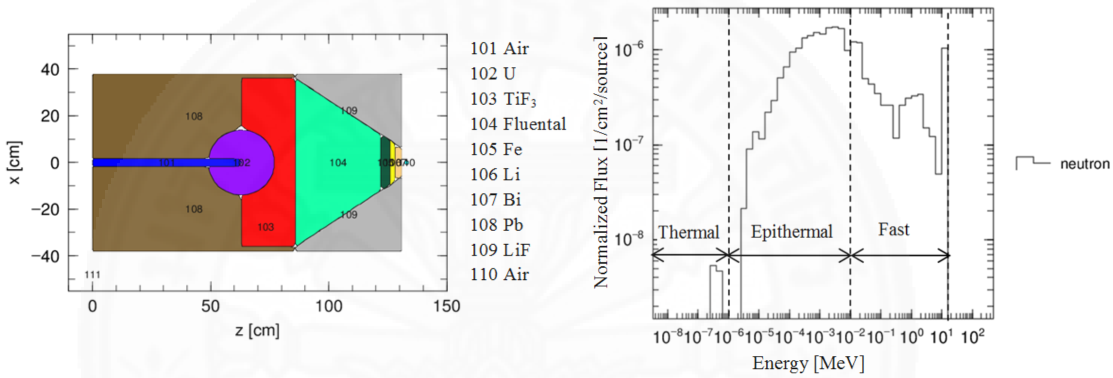
Figure 3.2 (a) presents the design B. This BSA design consists of metallic uranium as neutron multiplier, TiF_3 as first moderator, Al_2O_3 as second moderators, Pb as reflector, Ni as shield, and Li-Poly as collimator. The collimator is employed to guide neutrons toward the patient position. For the purpose of having a high epithermal neutron flux at the beam port, no filter is adopted in this design b. This design is able to produce an epithermal neutron flux of 3.67×10^9 n/cm^{2}s. Different from the design A, the thermal neutron flux (0.02×10^9 n/cm^{2}s) generated by the design B is much lower than the produced epithermal neutron flux. Even the fast neutron flux (0.47×10^9 n/cm^{2}s) is also lower than the epithermal neutron flux.



(a) **(b)**

Figure 3.2 The BSA design (a) and neutron beam port flux per neutron source versus energy proposed (b) proposed by Rasouli and Masoudi (Rasouli & Masoudi, 2012).

Figure 3.3 (a) shows the design C. It is composed of 14 cm U as multiplier, 23 cm TiF_3 as first moderator, 36 cm Fluental as second moderator, 4 cm Fe as fast neutron filter, 1 mm Li as thermal neutron filter, 2.6 cm Bi as gamma shield, Pb as collimator and reflector, LiF as shield. An epithermal neutron flux of 3.32×10^9 n/cm^2 s can be produced by this design. It is interesting to note that by adopting the thermal neutron filter, the generation of thermal neutron flux can be greatly suppressed. The design only generated 4×10^6 n/cm^{2}s of thermal neutron flux, which is much lower as compared to that of epithermal neutron flux.



(a) (b)

Figure 3. 3 The BSA design (a) and neutron beam port flux per neutron source versus energy (b) proposed by Rasouli et al. (Rasouli et al., 2012).

It can be seen in table 3.1 that, all the designs satisfy the International Atomic Energy Agency (IAEA) recommended value for epithermal neutron flux, in which the design B yields the highest value of φ_{epi} production. The values of epithermal flux are sufficient for BNCT.

Table 3. 1 BNCT in-air parameters of the three proposed BSA.

BSA design	φ_{epi} ($\times$ 10^9 n/cm^{2}s)	φ_{fast} ($\times$ 10^9 n/cm^{2}s)	φ_{therm} ($\times$ 10^9 n/cm^{2}s)	$\varphi_{epi}/\varphi_{fast}$	$\varphi_{epi}/\varphi_{therm}$
Design A (Eskandari & Kashian, 2009)	1.73	0.47	2.58	3.62	0.67
Design B (Rasouli & Masoudi, 2012)	3.67	2.65	0.02	1.38	179
Design C (Rasouli et al., 2012)	3.32	1.56	0.004	2.12	851
IAEA (Sauerwein et al., 2002)	>0.5			>20	>100

Although the design A uses two multiplication layers composing of Pb and U, it shows a lower value of φ_{epi} compared to the other two designs. This suggest that, adopting more than one layer as multiplier does not necessarily result in high φ_{epi} since the function of multiplier is to increase the number of all types of neutron emitted from neutron source.

It is interesting to note that, hypothetically, use of a second moderator can reduce the number of fast neutrons and thus increase $\varphi_{epi}/\varphi_{fast}$. However, although design B and design C use two moderator, the number of fast neutrons is surprisingly higher than that in the design A, which has one moderator. It seems that selecting a proper material for moderator is more important than adopting additional layers as moderator. It can also be seen that a relatively high number of fast neutrons in all three BSA designs is observed. This may be because U, as multiplier, can fairly intensify the number of fast neutrons (Faghihi & Khalili, 2013). In addition, due to gamma emission, U is also considered as unsuitable material for multiplier (Faghihi & Khalili, 2013).

Furthermore, TiF_3 was found to be an excellent material for a moderator in term of neutron accumulating in epithermal energy range during the slowing down from source energies. However, simulation results show unsuitability of TiF_3 as moderator in the design B and design C although a second moderator is also employed to reduce the number of fast neutrons.

Fig. 3.1b, Fig. 3.2b and Fig. 3.3b show the neutron flux per neutron source versus energy passing through the BSA. It can be seen that design A generates high thermal neutron flux, resulting in very low of $\varphi_{epi}/\varphi_{therm}$. The IAEA criterion of $\varphi_{epi}/\varphi_{therm}$ is thus unable to be satisfied. Further, design C shows a very low value of φ_{therm} because it uses Li filter for reducing the thermal neutron.

Overall, for BNCT in terms of $\varphi_{epi}/\varphi_{fast}$ and $\varphi_{epi}/\varphi_{therm}$, the most suitable designs are design A and C, respectively. Due to the fact that all the BSA designs can satisfy the IAEA criteria of φ_{epi} and the difference in the value of $\varphi_{epi}/\varphi_{therm}$ is also much more significant as compared to that of $\varphi_{epi}/\varphi_{fast}$, it suggested that design C is the most appropriate BSA design for BNCT. It is important to note that, however, none of those three BSA designs satisfies all the IAEA criteria.

Comparing the in-air parameters shown in Table 2.1 and Table 3.1, it is noticed that the values are not the same for design B and design C between the previously reported data and the present calculations. These differences in the in-air parameters are due to the slight differences in the BSA configurations, because the exact configuration of some BSA compounds are not provided in the previous reports.

Chapter 4
Development of BSA for BNCT

4.1 Introduction

The aim of this chapter was to develop a BSA design that is able to produce an epithermal neutron beam with the compact neutron generator based on D-D reactions for BNCT. An example of this type of neutron generator is a coaxial RF-driven plasma ion source, emitting monoenergetic neutrons with Nested Option (IB-1764) (Reijonen et al., 2005; Reijonen et al., 2002). The neutron source and BSA configuration were modeled with Particle Heavy and Ion Transport code System (PHITS) (Sato et al., 2013). The optimum condition for producing epithermal neutrons was used together with the IAEA standard of neutron beams for BNCT. Some existing BSA designs, i.e. those of Eskandari and Kashian (2009), Rasouli et al. (2012), and Rasouli and Masoudi (2012), were also simulated with PHITS for comparison. Finally, the output neutron beam characteristics were assessed based on the standard free beam parameters. The standard free beam parameters are proposed by the IAEA to define the quality of neutron beam on the beam port.

4.2. Materials and methods

A new design of BSA for a D-D nuclear fusion compact generator is proposed in this study. The simulated D–D neutron generator was assumed to produce fast neutrons with the energy of 2.45 MeV. In this work, it was assumed that the input fast neutron beam possessed a diameter of 1.7 cm with a neutron flux of 10^{13} n/s (Reijonen et al., 2005; Reijonen et al., 2002). A multiplier with cylindrical geometry composed of Pb was used as the first component to increase the neutron flux. In addition a large cross section of Pb for the (n, 2n) reaction can recompense neutron losses due to leakage and absorption (Cerullo et al., 2002). The second component was a moderator composed of TiF_3. TiF_3 was employed since materials containing fluorine showed the ability to effectively accumulate neutrons in the epithermal energy range during the moderation process (Eskandari & Kashian, 2009). The third component was a second moderator composed of AlF_3. By adopting a second moderator, the ratio between epithermal neutron flux and fast neutron flux ($\varphi_{epi}/\varphi_{fast}$)

is expected to increase due to increased epithermal neutron flux and decreased fast neutron flux. Further, a reflector composed of Al_2O_3 was placed around the multiplier and the moderators to reflect neutrons into the multiplier and/or the moderator region. Therefore, any leakages from these BSA regions could be minimized. Finally, Li was used as a thermal neutron filter since thermal neutrons are detrimental to the treatment process and are not desired at the surface of the patient. In order to obtain a suitable BSA, the proposed BSA design was developed to fulfill the IAEA recommendation for BNCT as shown in Table 4.1.

Table 4. 1 BNCT free beam parameters recommended by the IAEA (IAEA, 2001) φ represents neutron flux, n stands for neutron, and s stands for second

Beam port parameters	Recommended value
φ_{epi} (n/cm^2 s)	~0.5×10^9
$\varphi_{epi}/\varphi_{fast}$	>20
$\varphi_{epi}/\varphi_{thermal}$	>100

4.3 Results and discussion

As previously mentioned, BSA configuration should be appropriately optimized to yield suitable characteristics of output neutron beam in terms of quality and quantity. For this purpose, different materials for BSA were used and their configurations were optimized.

4.3.1 Optimization of BSA design

A multiplier was adopted to increase the neutron flux. The Pb multiplier was simulated with different thicknesses of 2, 4, 8, 10, and 12 cm. As seen in Figure 4.1, the epithermal neutron flux varied greatly with respect to the thickness of Pb. The Pb multiplier with a thickness of 4 cm was found to be the best choice for the multiplier. It produced the highest epithermal neutron flux of 2.75×10^{-7} 1/cm^2/source.

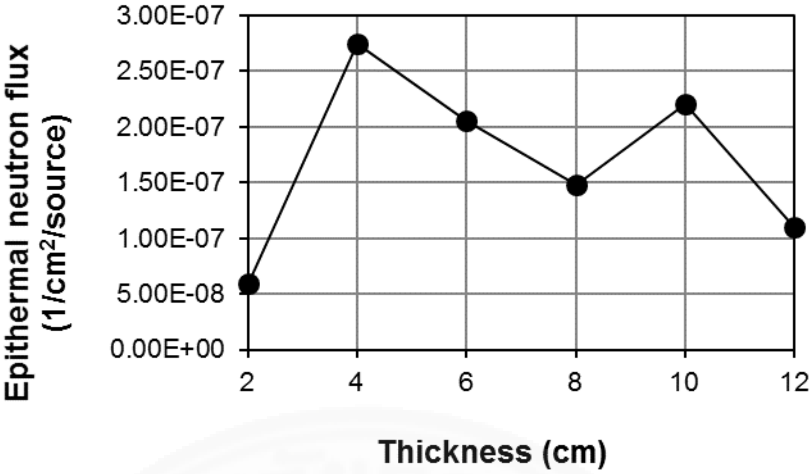


Figure 4. 1 Epithermal neutron flux per neutron source for different thicknesses of Pb as the multiplier.

In order to moderate the produced neutrons to the epithermal range after being multiplied by Pb, TiF_3 was adopted as the first moderator with 4 cm of Pb as the multiplier. Different thicknesses of TiF_3 ranging from 4 to 36 cm with an interval value of 4 cm were optimized. With increased thickness of TiF_3 from 4 cm to 20 cm, the epithermal neutron flux increased from 5.81×10^{-6} 1/cm^2/source to 1.16×10^{-4} 1/cm^2/source. Further increase of the TiF_3 thickness to 36 cm decreased the epithermal neutron flux to 4.95×10^{-5} 1/cm^2/source. As shown in Figure 4.2, insignificant difference of the epithermal flux between 16 and 20 cm of TiF_3 was observed. For this reason, 16 cm of TiF_3 was selected as the first moderator. By adopting 16 cm of TiF_3 as the moderator, the epithermal neutron flux was unfortunately still very low. This resulted in a very low value of $\varphi_{epi}/\varphi_{fast}$ of 4.94×10^{2}. To increase the value of $\varphi_{epi}/\varphi_{fast}$, a second moderator was further adopted.

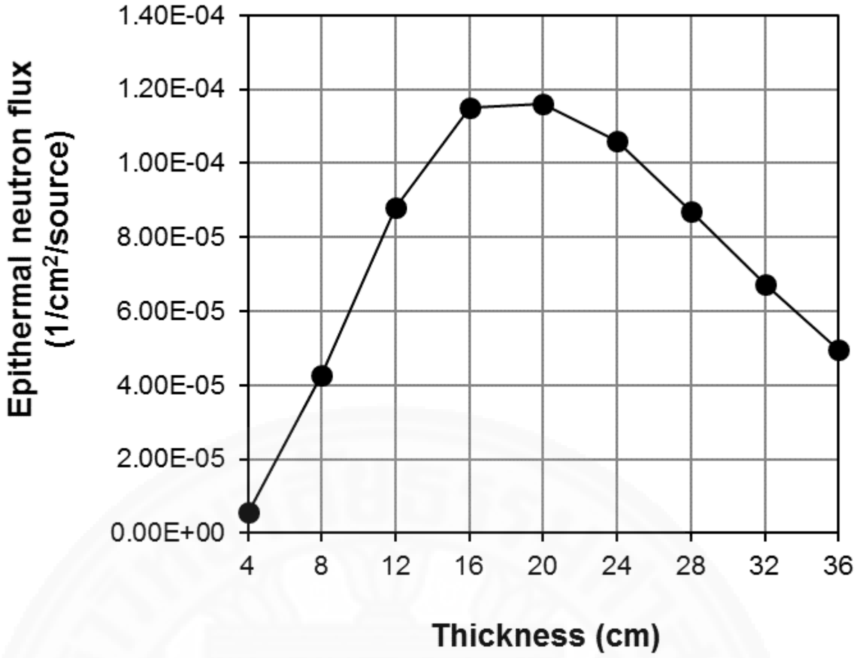


Figure 4. 2 Epithermal neutron flux per neutron source for different thicknesses of TiF_3 as the first moderator

For the second moderator, AlF_3 was adopted. Pb with 4 cm thickness and TiF_3 with 16 cm thickness were used as the multiplier and the first moderator, respectively. The trend of $\varphi_{epi}/\varphi_{fast}$ values was similar to that of epithermal neutron flux for the first moderator. That is, as the thickness of AlF_3 increases from 4 cm to 60 cm, $\varphi_{epi}/\varphi_{fast}$ increases from 9.77×10^{-2} to 24.6. With further increase of the AlF_3 thickness to 60 cm, $\varphi_{epi}/\varphi_{fast}$ drastically decreased to 6.27. Therefore, 60 cm of AlF_3 was chosen as the second moderator as shown in Figure 4.3. It was found that by adopting 60 cm of AlF_3 as the second moderator, the fast neutron flux was significantly reduced, indicated by a high value of $\varphi_{epi}/\varphi_{fast}$ of 24.6. Due to this fact, the fast neutron filter was not required for the proposed BSA design.

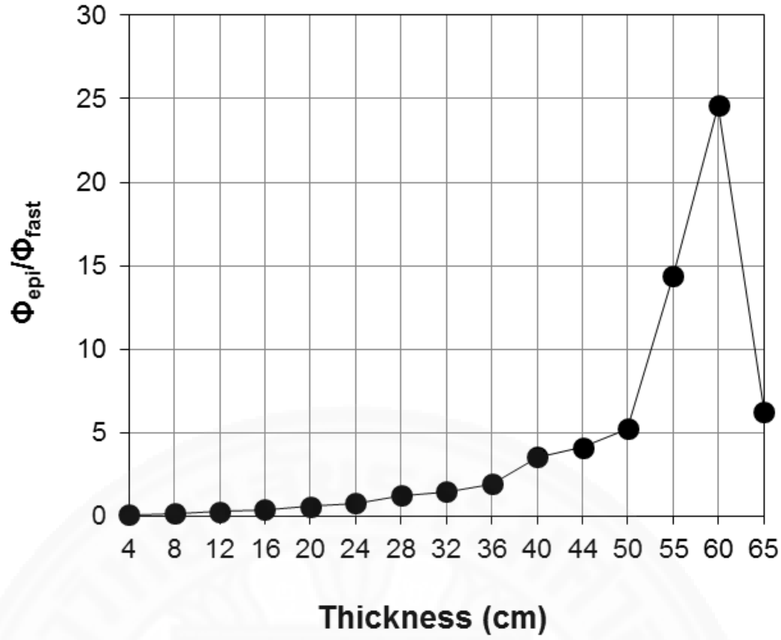


Figure 4. 3 $\varphi_{epi}/\varphi_{fast}$ for different thicknesses of AlF_3 as the second moderator.

To reflect the produced neutrons into the multiplier region and the moderator region, a reflector with Al_2O_3 was adopted. A configuration of 4 cm of Pb as the multiplier, 16 cm of TiF_3 as the first moderator, and 60 cm of AlF_3 as the second moderator was applied. Different thicknesses of Al_2O_3 (25, 30, and 35 cm) were evaluated to determine their reflective capabilities. The $\varphi_{epi}/\varphi_{fast}$ values for 25, 30, and 35 cm thickness of Al_2O_3 were calculated to be 17.8, 26.3, and 25.9, respectively. Thus, 30 cm of Al_2O_3 was adopted as the reflector. However, it should be noted that the $\varphi_{epi}/\varphi_{thermal}$ value of Al_2O_3 with 30 cm thickness was still relatively low and did not meet the IAEA's recommended value (Table 1). The $\varphi_{epi}/\varphi_{thermal}$ values for 25, 30, and 35 cm thickness of Al_2O_3 were 6.78, 3.3, and 2.61, respectively. This indicated that the thermal neutron flux was still high. Thermal neutrons are undesirable as they can introduce too high radiation dose to the soft tissue. For this reason, a thermal neutron filter was adopted.

For the purpose of reducing the thermal neutron flux and increasing the epithermal flux, Li was adopted as the thermal neutron filter. The natural Li possesses a large thermal neutron absorption cross section of 940 barns. A configuration of 4 cm of Pb as the multiplier, 16 cm of TiF_3 as the first moderator, 60 cm of AlF_3 as the second moderator, and 30 cm of Al_2O_3 as the reflector was used. Different thicknesses of Li (1, 2, 3, and 4 cm) were investigated to find the suitable thickness, indicated by the larger value of $\varphi_{epi}/\varphi_{thermal}$. As can be seen in Figure 4.4a, with the increase of Li thickness from 1 cm to 4 cm, the $\varphi_{epi}/\varphi_{thermal}$ value continuously increased from 26.2 to 174. All of these $\varphi_{epi}/\varphi_{thermal}$ values complied with the IAEA recommended value. Therefore, to select the most appropriate Li thickness, another free beam parameter for BNCT, namely, $\varphi_{epi}/\varphi_{fast}$ was considered. As shown in Figure 4.4b, 3 cm of Li exhibited the highest $\varphi_{epi}/\varphi_{fast}$ value of 27. Thus, 3 cm of Li was opted as the thermal neutron filter.

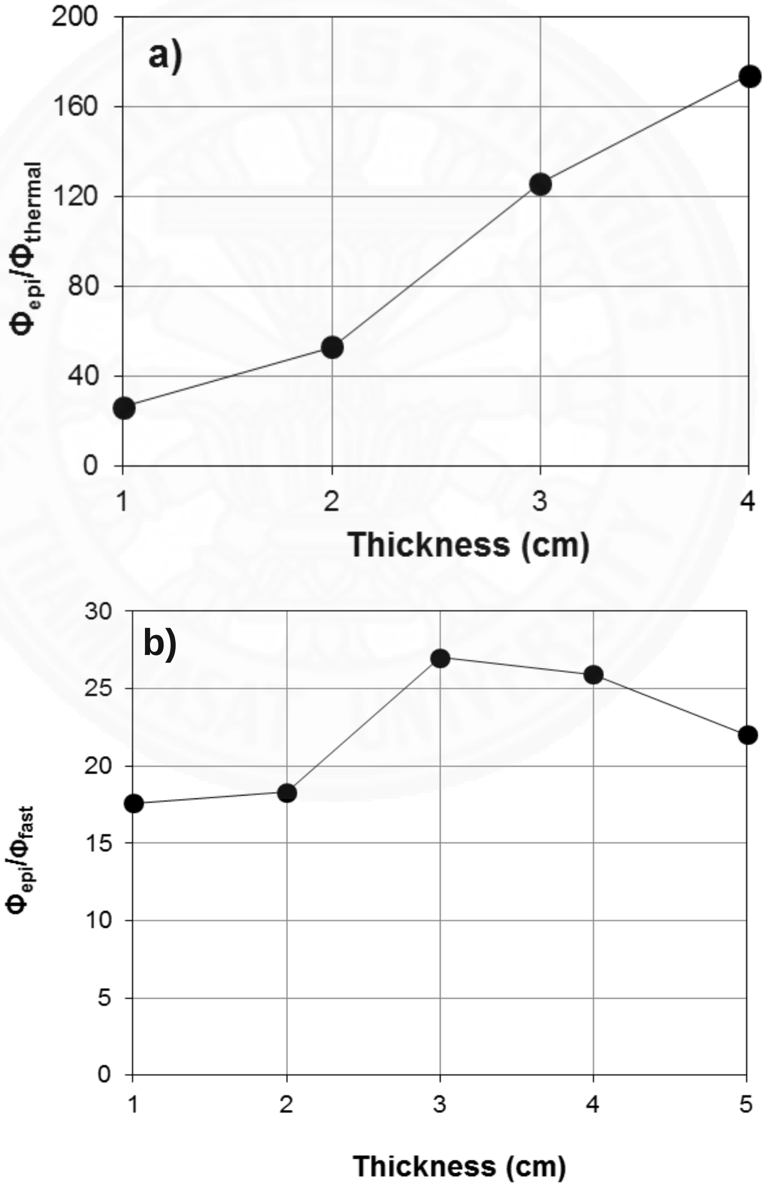
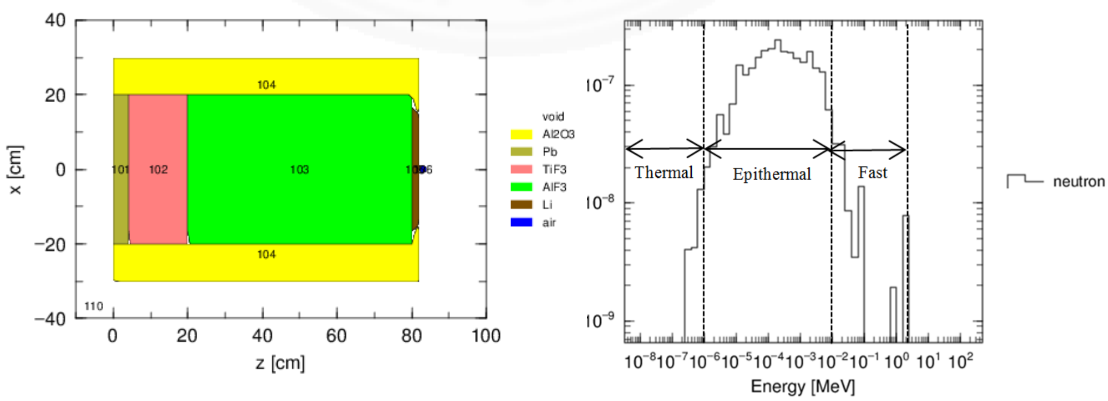


Figure 4. 4 $\varphi_{epi}/\varphi_{thermal}$ (a) and $\varphi_{epi}/\varphi_{fast}$ (b) for different thicknesses of Li as the thermal neutron filter.

Overall, the proposed BSA configuration for fast neutrons from a compact neutron source based on D-D nuclear fusion reactions consisted of 4 cm of Pb as the multiplier, 16 cm of TiF_3 as the first moderator, 60 cm of AlF_3 as the second moderator, 30 cm of Al_2O_3 as the reflector, and 3 cm of Li as the thermal filter (Figure 4.5a). The $\varphi_{epi}/\varphi_{fast}$ and $\varphi_{epi}/\varphi_{thermal}$ values of the proposed BSA, which represented the quality of the free beam parameters, were 27 and 126, respectively. The values of these parameters satisfied the IAEA recommended values for BNCT. The results showed that materials containing fluorine, which were adopted as the first moderator (TiF_3) and the second moderator (AlF_3), were suitable to increase the epithermal neutron flux. Additionally, by adopting materials containing fluorine, the fast neutron flux was significantly reduced. Thus, no fast neutron filter was needed for the proposed BSA design. Moreover, Li was proven to be a proper material choice to reduce the thermal neutron flux. Although the quality of the neutron beam was in agreement with the IAEA criteria, the intensity of epithermal neutrons was still below the recommended value. By taking a neutron yield of 10^{13} n/s generated from the simulated D-D neutron source, the epithermal neutron flux at the beam port of the proposed BSA facility was found to be only 2.66×10^{7} n/cm^{2}s (Figure 4.5b). This is because D-D neutron generators typically produce low neutron flux as compared to other neutron sources, such as nuclear reactors or D-T neutron generators. Improvement may be possible through material selection and source capacity enhancement.

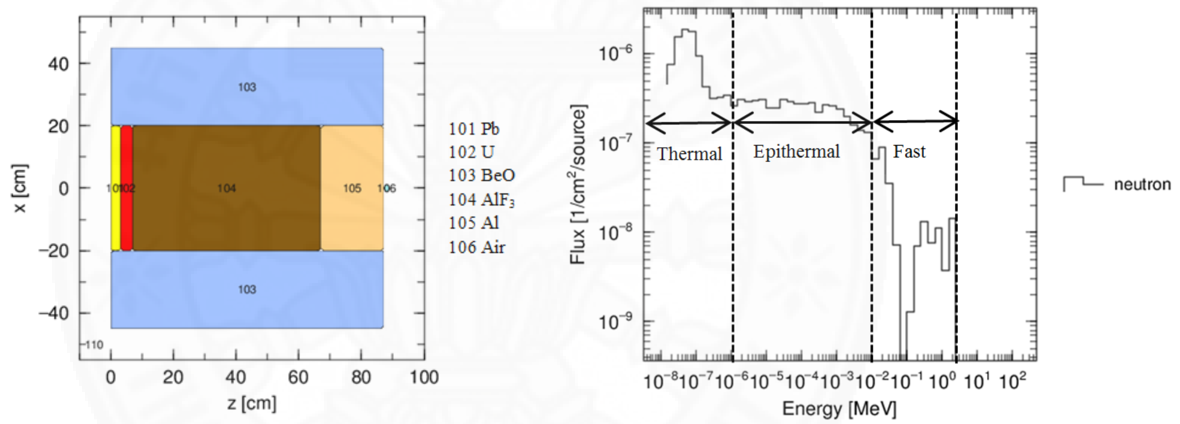


(a) (b)

Figure 4. 5 The proposed BSA design (a) and the neutron flux per neutron source at the beam port exit versus neutron energy (b).

4.3.2. Comparison of BSA designs

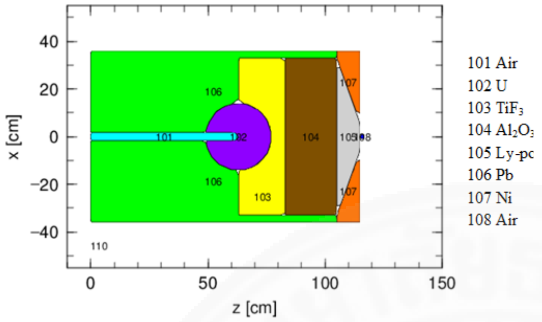
For the purpose of comparison, the BSA designs proposed by Eskandari and Kashian (2009), Rasouli et al. (2012), and Rasouli and Masoudi (2012), were also taken into consideration, which for the sake of simplicity were indicated as design A, design B, and design C, respectively. Figure 4.6a shows the design A, composed of 3 cm of Pb as the first multiplier, 2 cm of U as the second multiplier, 25 cm of BeO as the reflector, 60 cm of AlF_3 as the moderator, and 20 cm of Al as the fast filter. The out coming value of epithermal neutron flux was calculated to be 5.05 × 10^7 n/cm^2 s (Figure 4.6b). The $\varphi_{epi}/\varphi_{fast}$ and $\varphi_{epi}/\varphi_{therm}$ values of design A were 19.5 and 0.57, respectively. Therefore, no free beam parameter of design A was found to meet the IAEA recommended values.

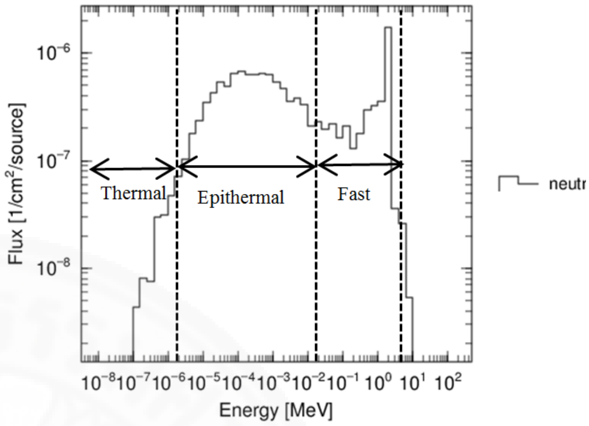


(a) (b)

Figure 4. 6 The BSA design A (a) and the neutron flux per neutron source at the beam port exit versus energy (b). The BSA design was proposed by Eskandari and Kashian (2009).

Figure 4.7a presents the design B, consisting of 14 cm of U as the neutron multiplier, 20 cm of TiF_3 as the first moderator, 22 cm of Al_2O_3 as the second moderator, 105 cm of Pb as the reflector, 69 cm of Ni as the gamma shield, and 10 cm of Li-Poly as the collimator. The collimator was used to guide neutrons toward the patient position. For obtaining a high epithermal neutron flux at the beam port exit, no filter was adopted in the design B. This BSA configuration could produce an epithermal neutron flux of 8.44 × 10^7 n/cm^2s. However, as seen in Figure 4.7b, the thermal neutron flux was much lower than the epithermal neutron flux. The similar trend was also found for the fast neutron flux. It was still lower than the epithermal neutron flux. As a result, the $\varphi_{epi}/\varphi_{fast}$ value of 1.95 was far from the IAEA's recommended value, while the $\varphi_{epi}/\varphi_{therm}$ value of 104 was only slightly higher than the recommended value.

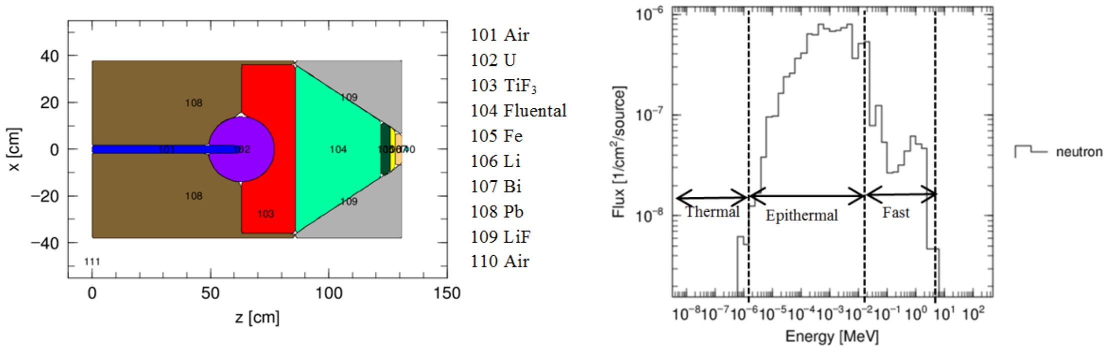




(a) (b)

Figure 4. 7 The BSA design B (a) and neutron flux per neutron source at the beam port exit versus energy proposed (b). The BSA design was proposed by Rasouli and Masoudi (2012).

Figure 4.8a shows the design C, composed of 14 cm of U as the multiplier, 23 cm of TiF_3 as the first moderator, 36 cm of Fluental as the second moderator, 4 cm of Fe as the fast neutron filter, 1 mm of Li as the thermal neutron filter, 2.6 cm of Bi as the gamma shield, Pb as the collimator and the reflector, and LiF as the neutron shield. The epithermal neutron flux of 7.74×10^7 n/cm^2 s could be produced by this BSA design (Figure 4.8b). By adopting Li as the thermal neutron filter, the generation of thermal neutron flux could be greatly suppressed. This led to a very high value of $\varphi_{epi}/\varphi_{thermal}$ of 1240. A similar result was also observed in our proposed BSA design. Adopting Li as the thermal neutron filter reduced the thermal neutron flux, resulting in a relatively high value of $\varphi_{epi}/\varphi_{thermal}$. Li seemed to be a suitable material choice for the thermal neutron filter. On the contrary, Fe was found to show a poor performance for removing fast neutrons, indicated by a low value of $\varphi_{epi}/\varphi_{fast}$ of 4.84.



(a) (b)

Figure 4. 8 The BSA design C (a) and neutron flux per neutron source at beam port exit versus energy (b). The BSA design was proposed by Rasouli et al. (2012).

Comparing the proposed BSA design with some other BSA designs developed by Eskandari and Kashian (2009), Rasouli et al. (2012), and Rasouli and Masoudi (2012), it was found that our design showed a better performance in terms of $\varphi_{epi}/\varphi_{fast}$. The value of $\varphi_{epi}/\varphi_{fast}$ also satisfied the IAEA criterion for $\varphi_{epi}/\varphi_{fast}$. Among all BSA designs investigated, the design C produced the highest value of $\varphi_{epi}/\varphi_{thermal}$, which was even much higher than the minimum value recommended by the IAEA. Furthermore, the design B showed the highest value of epithermal neutron flux since it had no thermal neutron filter. However, the epithermal neutron flux was still below the recommended value. The BNCT free beam parameters of the investigated BSA designs with the D-D neutron source are summarized in Table 4.2.

Table 4. 2 BNCT free beam parameters of each BSA designs for D-D neutrons

BSA design	φ_{epi} ($\times$ 10^7 n/cm^2 s)	$\varphi_{epi}/\varphi_{fast}$	$\varphi_{epi}/\varphi_{thermal}$
This work	2.66	27	126
Design A	5.05	19.5	0.57
Design B	8.44	1.9	104
Design C	7.74	4.8	1240
IAEA	>50	>20	>100

It is interesting to note that, although the design A used two multiplication layers composing of Pb and U, it showed a lower value of φ_{epi} compared to the design B and the design C. This suggested that, adopting more than one layer as a multiplier did not necessarily result in higher epithermal flux. Moreover, it is known that use of a second moderator typically leads to reduction of the number of fast neutrons and increased $\varphi_{epi}/\varphi_{fast}$. However, although the design B and the design C used two moderators, the number of fast neutrons was surprisingly higher than that of the design A, which had only a single moderator. Therefore, selecting a proper material as the moderator is more important than adopting additional layers as the moderator. Moreover, high numbers of fast neutrons; and thus low values of $\varphi_{epi}/\varphi_{fast}$, in the design A, the design, B, and the design C, were observed. This implied that, using U, as the multiplier, intensified the number of fast neutrons, which is detrimental to the neutron beam quality, and therefore U is unsuitable to be used as the multiplier material. Employing Pb as the multiplier material seemed to be promising, as it was evidenced in the proposed BSA design. The $\varphi_{epi}/\varphi_{fast}$ value of 27 of the proposed BSA satisfied the IAEA value for BNCT.

Overall, by using the proposed BSA design as well as the design C, the quality of neutron beam was satisfying. However, the quantity of the epithermal neutron still need to be enhanced as no BSA designs satisfied the recommended value for BNCT. The low quantity of epithermal neutrons was due to the relatively low D-D neutron output of only 10^{13} n/s. Similar results on the BSA designs based on D-D neutron generators were also reported (Durisi et al., 2007; Fantidis et al., 2013). The epithermal neutron flux produced by those BSA designs was also below the IAEA recommended value for clinical treatment.

Chapter 5
Conclusion

5.1 Conclusion

Three existing BSA designs were evaluated to moderate fast neutron from D-T neutron source for BNCT. They have φ_{epi} values satisfying the IAEA criteria. According to the simulations and performed calculations, the BSA design proposed by Rasouli et al. (2012) yields the best performance. It produces epithermal neutron flux of 3.32×10^9 n/cm^2 s in the range suggested by the IAEA and $\varphi_{epi}/\varphi_{fast}$ of 851 and efficiently reduces fast neutron into appropriate level. Moreover, it exhibits a very low value of φ_{therm} since it uses Li filter for reducing the thermal neutron. With the same design using D-D neutron source, an epithermal neutron flux of 7.74×10^7 n/cm^2 s and $\varphi_{epi}/\varphi_{fast}$ of 4.8 can be produced. Interestingly, a very high $\varphi_{epi}/\varphi_{thermal}$ of 1240 is obtained. However, none of those three BSA design satisfies all the IAEA criteria.

A new BSA design for slowing down fast neutrons to the epithermal energy range from a D-D neutron generator was furthermore designed for BNCT. An optimum design of BSA consisted of 4 cm of Pb as the multiplier, 16 cm of TiF_3 as the first moderator, 60 cm of AlF_3 as the second moderator, 30 cm of Al_2O_3 as the reflector, and 3 cm of Li as the thermal filter. The proposed BSA with the D-D neutron generator with a neutron yield of 10^{13} n/s produced an epithermal neutron flux of 2.66×10^7 n/cm^2 s, $\varphi_{epi}/\varphi_{fast}$ of 27, and $\varphi_{epi}/\varphi_{thermal}$ of 126. The obtained values of free beam parameters satisfied those recommended by IAEA, except the epithermal neutron flux. This was because D-D neutron generators produce relatively low neutron flux as compared to nuclear reactors and D-T neutron generators. Despite this fact, D-D neutron generators were shown to be applicable for achieving appropriate quality of neutron beam and thus the proposed BSA design with an improved performance of D-D neutron generators could be applied for BNCT purpose. In order to achieve the minimum quantity of neutron flux required for BNCT, one should employ, or develop if it has not yet been available, a D-D neutron generator capable of producing a neutron yield of more than 10^{15} n/s.

5.2 Recommendation and future work

- To obtain BSA with better performance which can satisfy all the IAEA criteria, more parameters such as geometry and type of material need to be further investigated.
- To obtain more comprehensive results, the angular energy spectra need to be measure. For this purpose, the neutron angular distribution at different angle should be measured.
- To realize more effective BSA design, in-phantom parameters need to be determined, besides in-air parameters.
- To be able to use the proposed BSA design with satisfied results in term of both quality and quantity of the neutron flux, a D-D neutron generator capable of producing a neutron yield of more than 10^{15} n/s should be employed.

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Appendices

Appendix A

Comparison of Existing Design

1. The BSA design proposed by Eskandari and Kashian
1.1. Input file

```
[title]
Example 1: Get started
$ "D" = default value
$ Comments with '$', '#', 'c'

$
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%
[parameters]          $ Simulation parameters
file(6)  = phits.out  $ Output filename
maxcas   = 1e7        $ Number of events per batch
maxbch   = 1          $ Number of batch
imout    = 2          $ Option of material representation in [material] 2:MCNP-type
icntl    = 0          $ (D=0)Calculation mode: 0=real simulation, 5=no reactions
(void all), 6=source check, 8=check geometry
itall    = 1          $ (D=0) Tally ouput after every batch. D=0 not output, D=1
output in same file

$ Cut-off energy
emin(1)  = 1.0e-3     $ (D=1.0) cut-off energy for proton (MeV)
emin(2)  = 1.e-10     $ (D=1.0) cut-off energy for neutron (MeV)
emin(12) = 1.e-1      # (D=1.d9) cut-off energy of electron (MeV)
emin(13) = 1.e-1      # (D=1.d9) cut-off energy of positron (MeV)
emin(14) = 1.e-3      # (D=1.d9) cut-off energy of photon (MeV)
emin(15) = 2.0e-3     # (D=1.d9) cut-off energy of deuteron (MeV/nucleon)
emin(16) = 3.0e-3     # (D=1.d9) cut-off energy of triton (MeV/nucleon)
emin(17) = 3.0e-3     # (D=1.d9) cut-off energy of 3He (MeV/nucleon)
emin(18) = 4.0e-3     # (D=1.d9) cut-off energy of Alpha (MeV/nucleon)
emin(19) = 1.0e-3     # (D=1.d9) cut-off energy of Heavy Ion (MeV/nucleon)

$ Maximum energy of nulcear data library used
$ By default, PHITS omits electron/positron/photon transport & uses Boltzmann
transport for low-energy neutrons (<20MeV)
dmax(2)  = 20.0           $ Neutron
dmax(12) = 1.0            $ Electron
dmax(13) = 1.0            $ positron
dmax(14) = 1.0            $ photon
```

$ Option for nuclear reactions
e-mode = 1 $ (D=0) Option for event-generator: 0=OFF, 1=ON
igamma = 1 $ (D=0) Option for gamma decay for residual nuclei: 0=no decay, 1=use 'trxcrd.dat', 2=EBITIM model, 3=EBITIM+isomer production
ipnint = 1 $ (D=0) Option for photonuclear reaction: 0=OFF, 1=ON
file(7) = data/xsdir.jnd $ Cross section data library for low energy neutrons
file(14)= data/trxcrd.dat $ Cross section data library for photon emission from residual nuclei

$ Option for charged particle transport
nedisp = 1 $ (D=0) Energy straggling: 0=OFF, 1=Landau-Vavilov
nspred = 2 $ (D=0) Angle straggling: 0=OFF, 2=Moliere First Coulomb diffusion
itstep = 1 $ (D=0) Option for timing tally "correct" curvature for momentum changing trajectory e.g. in magnetic field

$
%%
%%%%%%%%%%%
[source]
s-type = 1 % Source type: 1=cylinder, 2=rectangular, 9=spherical
proj = 2112 % Projectile: 2112=neutron
dir = 1 % Initial direction relative to positive-z axis: dir=cosine
e0 = 14.1 % Initial energy (MeV)

x0 = 0
y0 = 0
z0 = -1. % zmin (cm)
z1 = -1. % zmax: z1=z0 circle plan source
r0 = 1.7 % radius of the cylindrical source

$
%%
%%%%%%%%%%%
[material]
$ Material composition info: nuclei & density
$ Density can be defined in [cell], then in [material] you only need to define material compositions
$ i.e. weight fractions, if density is defined in g/cm^3, or atomic fractions if density in 10^24 atoms/cm^3
$ Library number and data class in "data/xsdir.jnd"

MAT[1] $ Lead, den = 11.35 g/cc
82204.50c -0.01378
82206.50c -0.23955
82207.50c -0.22074
82208.50c -0.52592

```
MAT[2] $ Uranium 238, den = 18.95g/cc
         92234.50c      -0.000057
          92235.50c      -0.007204
         92238.50c      -0.992739

MAT[3] $ Beryllium Oxide, den = 3.01 g/cc
         4009.50c       -0.360320
         8016.50c       -0.639680

MAT[4] $ Aluminium Fluoride, den = 2.88 g/cc
         13027.50c          -0.32130
         9019.50c       -0.67870

MAT[5] $ Aluminium, den=  2.6989 g/cc
         13027.50c          -1.0000

MAT[6] $ Dry air, den=0.001205g/cc
        6000.50c              -0.000124
        7014.50c              -0.752291
        7015.50c              -0.002977
        8016.50c              -0.231781
        18040.50c         -0.012827


$
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
[mat name color]
mat     name            size     color
0         void             1         white
1         Pb               1         yellow
2        U                 1      red
3       BeO               1      pastelblue
4      AlF3               1      brown
5      Al                  1      pastelpink
6      Air                 1      pastelcyan

$
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
[ S u r f a c e ]
  10  so     500.
  11  cz       20.            $ Pb
  12  pz        0.            $ Pb
  13  pz        3.            $ Pb
  14  cz       20.            $ U
```

```
  15  pz       3.            $ U
  16  pz       7.            $ U
  17  cz      45.            $ BeO
  18  pz      0.             $ BeO
  19  pz      87.            $ BeO
  20  cz      20.            $ Alf3
  21  pz      7.             $ AlF3
  22  pz      67.            $ AlF3
  23  cz      20.            $ Al
  24  pz      67.            $ Al
  25  pz      87.            $ Al
  26  sph      0 0 0 1.       $ sphere radius 1 cm

$
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
[cell]
$ If density is positive: unit 10^24 atoms/cm^3 (= atoms/barn/cm)
$ If density is negative: unit g/cm^3

$id    mat    den             surface
 100   -1      10
  101   1       -11.35        -11  12  -13
  102   2       -18.95        -14  15  -16
  103   3       -3.01          -17  18  -19 #101 #102 #104 #105
  104   4       -2.88          -20  21  -22
  105   5       -2.6989        -23  24  -25
  106   6       -0.001205      -26         trcl=(0 0 88)              $ detector
  110   0       -10           #101  #102 #103   #104 #105  #106          $ working area

 $
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
 [volume]
 reg              vol
 101              3.768e3                 $ cell 1
 102          5.024e3       $ cell 2
 103          4.439175e5     $ cell 3
 104          7.536e4       $ cell 4
 105          2.512e4       $ cell 5
 106          4.19         $ cell 6


$
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
[ T - product ]off       $ Check product-eng
```

```
mesh    = reg
reg     = {101-105}

e-type  = 3                              $ (=3) log scale
ne      = 50
emin    = 1.e-8
emax    = 100.                           $ MeV

mother  = all

part    = Neutron Photon
unit    = 1                              $ 1/source

axis   =  eng
file   =  product-eng.dat
gshow  =  3
epsout =  1
resol  =  1

[t-track] off           $xy: check geometry
$Region crossing tally

mesh   = xyz

z-type = 1
nz     = 3
         -5 0 10 20 30 45

x-type = 2
nx     = 100
xmin   = -15
xmax   = 15

y-type = 2
ny     = 100
ymin   = -15
ymax   = 15

e-type = 3                               $ All energies
ne     = 1
emin   = 1e-8
emax   = 1e2                             $ MeV

part   = Neutron Photon                         $ 2112=neutron 22=photon
unit   = 1                               $ 1/cm^2/source
```

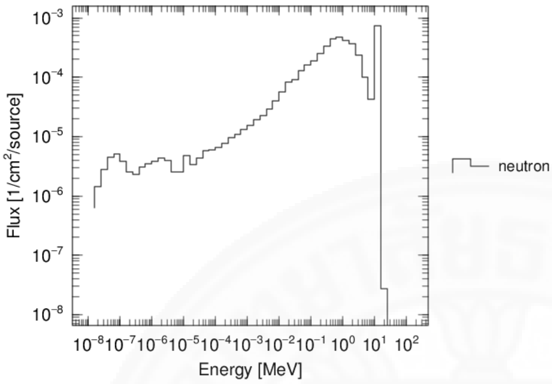
```
axis   = xy
file   = track-xy.dat                    $ all particles in one diagram
gshow  = 3                               $ 2: region boundary & material name; 3: region
boundary and name
epsout = 1
resol  = 1

$
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%
[t-track] off               $yz: check geometry
$Region crossing tally

mesh   = xyz

x-type = 1
nx     = 3
          -5 -0 +30 +50

y-type = 2
ny     = 100
ymin   = -50
ymax   = 50

z-type = 2
nz     = 100
zmin   = -5
zmax   = 100

e-type = 3                               $ All energies
ne     = 1
emin   = 1e-8
emax   = 1e2                             $ MeV

part   = Neutron                         $ 2112=neutron 22=photon
unit   = 1                               $ 1/cm^2/source

axis   = yz
file   = track-yz.dat                    $ all particles in one diagram
gshow  = 3                               $ 2: region boundary & material name; 3: region
boundary and region name
epsout = 1
resol  = 1

$
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%
```

```
[T-track]                    $ Tally particle energies in detectors
$ Region crossing tally

mesh    = reg
reg     = {101-106}
e-type  = 3                  $ (=3) log scale
ne      = 50
emin    = 1.e-8
emax    = 100.               $ MeV

part    = Neutron            $ 2112=neutron, 22=photon, 2212=proton
unit    = 1                  $ 1/cm^2/source

axis    = eng
file    = track-reg-eng-1e7.dat      $ all particles in one diagram
gshow   = 3                  $ 2: region boundary & material name; 3: region
boundary and name
epsout  = 1
resol   = 1

$
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%
[ T - product ]  off      $ Check source xy

mesh   = xyz

z-type = 1
nz     = 3
          -5 0 10 20 30 45

x-type = 2
nx     = 100
xmin   = -30
xmax   = 30

y-type = 2
ny     = 100
ymin   = -30
ymax   = 30

e-type = 3                   $ All energies
ne     = 1
emin   = 1.e-8
emax   = 100.0               $ MeV

part   =  neutron
```

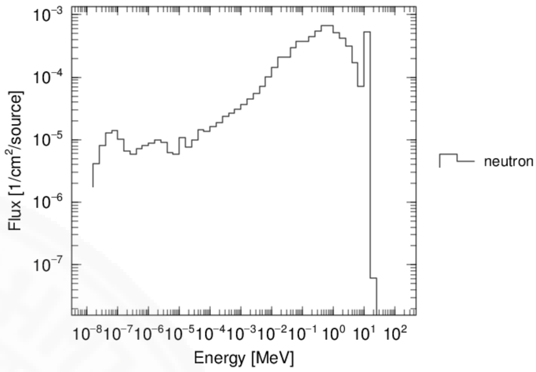
```
unit   =  1                                    $ (=1) 1/source, (=2) 1/cm^3/source
output =  source

axis   =  xy
file   =  source-xy.dat
gshow  =  3
epsout =  1
resol  =  1

[ T - Gshow ]  off
    mesh =  xyz           # mesh type is xyz scoring mesh
  x-type =    2           # x-mesh is linear given by xmin, xmax and nx
      nx =   50           # number of x-mesh points
    xmin =  -50.          # minimum value of x-mesh points
    xmax =   50.          # maximum value of x-mesh points
  y-type =    2           # y-mesh is linear given by ymin, ymax and ny
      ny =   50           # number of y-mesh points
    ymin =  -50.          # minimum value of y-mesh points
    ymax =   50.          # maximum value of y-mesh points
  z-type =    1           # z-mesh is given by the below data
      nz =    1           # number of z-mesh points
          0.0  45.0
    axis =   xy           # axis of output
  output =    6           # (D=2) 1:bnd, 2:bnd+mat, 3:bnd+num 4:bnd+mat+num
    file = xy_gshow.dat   # file name of output for the above axis
   title = Check geometry using [T-gshow] tally
  epsout =    1           # (D=0) generate eps file by ANGEL

[ T - Gshow ] off
    mesh =  xyz           # mesh type is xyz scoring mesh
  x-type =    2           # x-mesh is linear given by xmin, xmax and nx
      nx =   50           # number of x-mesh points
    xmin =  -55.          # minimum value of x-mesh points
    xmax =   55.          # maximum value of x-mesh points
  y-type =    1           # y-mesh is given by the below data
      ny =    1           # number of y-mesh points
          -55.0  55.0
  z-type =    2           # z-mesh is linear given by zmin, zmax and nz
      nz =   50           # number of z-mesh points
    zmin =  -10.          # minimum value of z-mesh points
    zmax =   100.         # maximum value of z-mesh points
    axis =   xz           # axis of output
  output =    6           # (D=2) 1:bnd, 2:bnd+mat, 3:bnd+num 4:bnd+mat+num
    file = xz_gshow.dat   # file name of output for the above axis
   title = Check geometry using [T-gshow] tally
  epsout =    1           # (D=0) generate eps file by ANGEL
```

$
%%
%%%%%%%%%%%
[end]

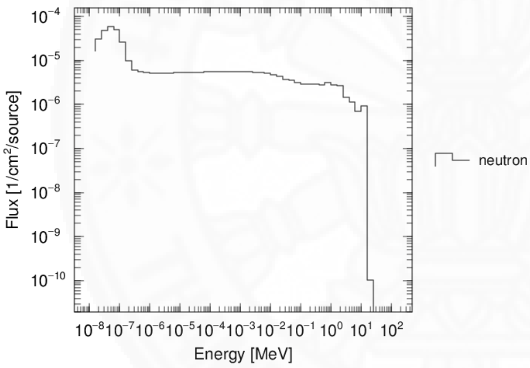
1.2. [T-Track] in region mesh



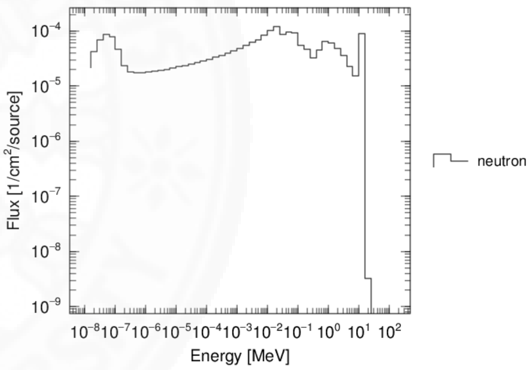
Reg = 101 Pb



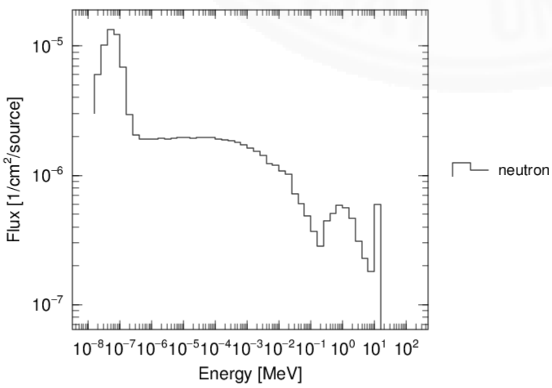
Reg = 102 U



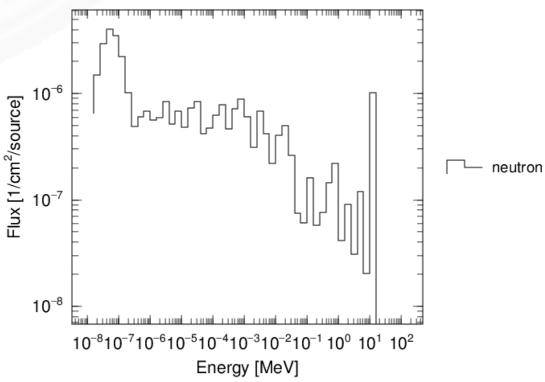
Reg = 103 BeO



Reg = 104 AlF3



Reg = 105 Al



Reg = 106 Air

2. The BSA design proposed by Rasouli and Masoudi

2.1. Input file

```
[title]
Example 1: Get started
$ "D" = default value
$ Comments with '$', '#', 'c'

$
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%
[parameters]            $ Simulation parameters
file(6)  = phits.out    $ Output filename
maxcas   = 1e7          $ Number of events per batch
maxbch   = 1            $ Number of batch
imout    = 2            $ Option of material representation in [material] 2:MCNP-type
icntl    = 0            $ (D=0)Calculation mode: 0=real simulation, 5=no reactions
(void all), 6=source check, 8=check geometry
itall    = 1            $ (D=0) Tally ouput after every batch. D=0 not output, D=1
output in same file

$ Cut-off energy
emin(1)  = 1.0e-3       $ (D=1.0) cut-off energy for proton (MeV)
emin(2)  = 1.e-10       $ (D=1.0) cut-off energy for neutron (MeV)
emin(12) = 1.e-1        # (D=1.d9) cut-off energy of electron (MeV)
emin(13) = 1.e-1        # (D=1.d9) cut-off energy of positron (MeV)
emin(14) = 1.e-3        # (D=1.d9) cut-off energy of photon (MeV)
emin(15) = 2.0e-3       # (D=1.d9) cut-off energy of deuteron (MeV/nucleon)
emin(16) = 3.0e-3       # (D=1.d9) cut-off energy of triton (MeV/nucleon)
emin(17) = 3.0e-3       # (D=1.d9) cut-off energy of 3He (MeV/nucleon)
emin(18) = 4.0e-3       # (D=1.d9) cut-off energy of Alpha (MeV/nucleon)
emin(19) = 1.0e-3       # (D=1.d9) cut-off energy of Heavy Ion (MeV/nucleon)

$ Maximum energy of nulcear data library used
$ By default, PHITS omits electron/positron/photon transport & uses Boltzmann
transport for low-energy neutrons (<20MeV)
dmax(2)  = 20.0               $ Neutron
dmax(12) = 1.0                $ Electron
dmax(13) = 1.0                $ positron
dmax(14) = 1.0                $ photon

$ Option for nuclear reactions
e-mode  = 1             $ (D=0) Option for event-generator: 0=OFF, 1=ON
igamma  = 1             $ (D=0) Option for gamma decay for residual nuclei: 0=no
decay, 1=use 'trxcrd.dat', 2=EBITIM model, 3=EBITIM+isomer production
ipnint  = 1             $ (D=0) Option for photonuclear reaction: 0=OFF, 1=ON
file(7) = data/xsdir.jnd      $ Cross section data library for low energy neutrons
```

file(14)= data/trxcrd.dat $ Cross section data library for photon emission from residual nuclei

$ Option for charged particle transport
nedisp = 1 $ (D=0) Energy straggling: 0=OFF, 1=Landau-Vavilov
nspred = 2 $ (D=0) Angle straggling: 0=OFF, 2=Moliere First Coulomb diffusion
itstep = 1 $ (D=0) Option for timing tally "correct" curvature for momentum changing trajectory e.g. in magnetic field

$
%%%
[source]
s-type = 1 % Source type: 1=cylinder, 2=rectangular, 9=spherical
proj = 2112 % Projectile: 2112=neutron
dir = 1 % Initial direction relative to positive-z axis: dir=cosine
e0 = 14.1 % Initial energy (MeV)

x0 = 0
y0 = 0
z0 = -1. % zmin (cm)
z1 = -1. % zmax: z1=z0 circle plan source
r0 = 1.7 % radius of the cylindrical source

$
%%%
[material]
$ Material composition info: nuclei & density
$ Density can be defined in [cell], then in [material] you only need to define material compositions
$ i.e. weight fractions, if density is defined in g/cm^3, or atomic fractions if density in 10^24 atoms/cm^3
$ Library number and data class in "data/xsdir.jnd"

MAT[1] $ Dry air, den=0.001205g/cc
6000.50c -0.000124
7014.50c -0.752291
7015.50c -0.002977
8016.50c -0.231781
18040.50c -0.012827

MAT[2] $ Uranium 238, den = 18.95g/cc
92234.50c -0.000057
92235.50c -0.007204
92238.50c -0.992739

```
MAT[3] $  Titanium trifluoride, den = 3.4 g/cc
           22048.50c         -0.336517056
           22046.50c         -0.037655035
           22049.50c         -0.024691003
           22047.50c         -0.033948418
           22050.50c         -0.023668488
           9019.50c          -0.54352

MAT[4] $ Aluminum Oxide, den = 3.97 g/cc
        8016.50c          -0.470749
        13027.50c          -0.529251

MAT[5] $ Lithiated Polyethylene (Li-Poly), den=  1.923513 g/cc
        3006.50c              -0.017437
        3007.50c              -0.215053
        6000.50c              -0.196334
        8016.50c              -0.561821
        1001.50c              -0.009354
        1002.50c              -0.000001

MAT[6] $ Lead, den = 11.35 g/cc
        82204.50c             -0.01378
        82206.50c             -0.23955
        82207.50c             -0.22074
        82208.50c             -0.52592

 MAT[7] $ Nickel, den= 8.902 g/cc
        28058.50c             -6.71977E-01
        28060.50c             -2.67760E-01
        28061.50c             -1.18336E-02
        28062.50c             -3.83482E-02
        28064.50c             -1.00815E-02

MAT[8] $ Dry air, den=0.001205g/cc
       6000.50c               -0.000124
       7014.50c               -0.752291
       7015.50c               -0.002977
       8016.50c               -0.231781
       18040.50c          -0.012827


$
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
[mat name color]
mat    name            size     color
```

```
 0         void               1          white
 1          air              1           cyan
 2         U                  1          violet
 3         TiF3              1           yellow
 4         Al2O3            1           brown
 5          Ly-Poly        1            gray
 6         Pb                1           green
 7         Ni                1           orange
 8         air              1          blue

 $
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%
  [transform]

  set: c10[0]     $ angle around Z (degree)
  set: c20[0]      $ angle around Y (degree)
  set: c30[0]      $ angle around X (degree)
  tr1
         +0 0 105
         cos(c10/180*pi)*cos(c20/180*pi)

         sin(c10/180*pi)*cos(c30/180*pi)+cos(c10/180*pi)*sin(c20/180*pi)*sin(c30/1
80*pi)
         sin(c10/180*pi)*sin(c30/180*pi)-
cos(c10/180*pi)*sin(c20/180*pi)*cos(c30/180*pi)
         -sin(c10/180*pi)*cos(c20/180*pi)
         cos(c10/180*pi)*cos(c30/180*pi)-
sin(c10/180*pi)*sin(c20/180*pi)*sin(c30/180*pi)

         cos(c10/180*pi)*sin(c30/180*pi)+sin(c10/180*pi)*sin(c20/180*pi)*cos(c30/1
80*pi)
         sin(c20/180*pi)
         -cos(c20/180*pi)*sin(c30/180*pi)
         cos(c20/180*pi)*cos(c30/180*pi)
         1

$
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%
[ S u r f a c e ]
  10  so      500.
  11  cz      1.7                    $ air
  12  pz      0.                     $
  13  pz      63.                    $
  14  sph      0 0 63. 14.           $ U
  15  cz       33.                   $ TiF3
```

```
  16  pz          63.                     $
  17  pz           83.                    $
  18  cz          33.                     $ Al2O3
  19  pz          83.                     $
  20  pz          105.                    $
  21  TRC         0 0 0 0 0 10 33 6       $ Ly-Poly
  22  cz          36.                     $ Pb
  23  pz           0.                     $
  24  pz          105.                    $
  25  cz          36.                     $ Ni
  26  pz          105.                    $
  27  pz          115.                    $
  28  sph         0 0 0 1.                $ sphere radius 1 cm

$
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%
[cell]
$ If density is positive: unit 10^24 atoms/cm^3 (= atoms/barn/cm)
$ If density is negative: unit g/cm^3

$id    mat    den              surface
  100   -1      10
  101   1       -0.001205    -11  12  -13
  102   2       -18.95         -14                               #101
  103   3       -3.4            -15  16  -17                     #102
  104   4       -3.97           -18  19  -20
  105   5       -1.923513    -21          trcl=1
  106   6       -11.35          -22  23  -24                    #101  #102 #103 #104
  107   7       -8.902          -25  26 -27                      #105
  108   8       -0.001205     -28          trcl=(0 0 116)         $ detector
  110   0        -10                         #101   #102 #103    #104 #105   #106 #107 #108
$ working area

 $
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%
[volume]
reg              vol
101            571.69              $ cell 1
102           11488.21
103           62645.09
104           75228.12
105           13847.4
106           277358.07
107           26847.
108           4.1
```

```
$
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%
[ T - product ]off        $ Check product-eng

mesh    = reg
reg     = {101-105}

e-type  = 3                          $ (=3) log scale
ne      = 50
emin    = 1.e-8
emax    = 100.                       $ MeV

mother  = all

part    = Neutron Photon
unit    = 1                          $ 1/source

axis   =  eng
file   =  product-eng.dat
gshow  =  3
epsout =  1
resol  =  1

[t-track] off             $xy: check geometry
$Region crossing tally

mesh   = xyz

z-type = 1
nz     = 3
         -5 0 10 20 30 45

x-type = 2
nx     = 100
xmin   = -150
xmax   = 150

y-type = 2
ny     = 100
ymin   = -150
ymax   = 150

e-type = 3                           $ All energies
ne     = 1
emin   = 1e-8
emax   = 1e2                         $ MeV
```

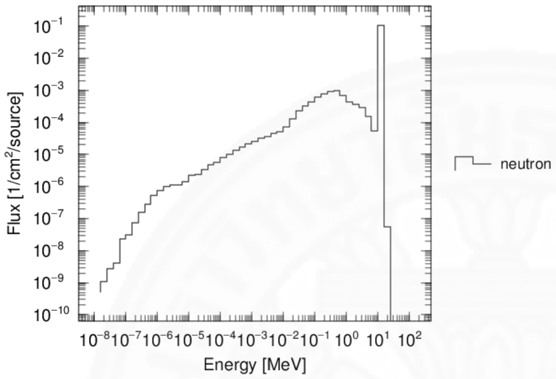
```
part   = Neutron Photon                    $ 2112=neutron 22=photon
unit   = 1                          $ 1/cm^2/source

axis   = xy
file   = track-xy.dat               $ all particles in one diagram
gshow  = 3                          $ 2: region boundary & material name; 3: region
boundary and name
epsout = 1
resol  = 1

$
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%
[t-track] off           $yz: check geometry
$Region crossing tally

mesh   = xyz

x-type = 1
nx     = 3
        -150 -0 +30 +150

y-type = 2
ny     = 100
ymin   = -150
ymax   = 150

z-type = 2
nz     = 100
zmin   = -150
zmax   = 150

e-type = 3                          $ All energies
ne     = 1
emin   = 1e-8
emax   = 1e2                        $ MeV

part   = Neutron                    $ 2112=neutron 22=photon
unit   = 1                          $ 1/cm^2/source

axis   = yz
file   = track-yz.dat               $ all particles in one diagram
gshow  = 3                          $ 2: region boundary & material name; 3: region
boundary and region name
epsout = 1
resol  = 1
```

```
$
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%
[T-track]                    $ Tally particle energies in detectors
$ Region crossing tally

mesh    = reg
reg     = {101-108}
e-type  = 3                           $ (=3) log scale
ne      = 50
emin    = 1.e-8
emax    = 100.                        $ MeV

part    = Neutron              $ 2112=neutron, 22=photon, 2212=proton
unit    = 1                           $ 1/cm^2/source

axis    = eng
file    = track-reg-eng-27e7.dat                $ all particles in one diagram
gshow   = 3                           $ 2: region boundary & material name; 3: region
boundary and name
epsout  = 1
resol   = 1

$
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%
[ T - product ]  off      $ Check source xy

mesh   = xyz

z-type = 1
nz     = 3
         -5 0 10 20 30 45

x-type = 2
nx     = 100
xmin   = -30
xmax   = 30

y-type = 2
ny     = 100
ymin   = -30
ymax   = 30

e-type = 3                            $ All energies
ne     = 1
```

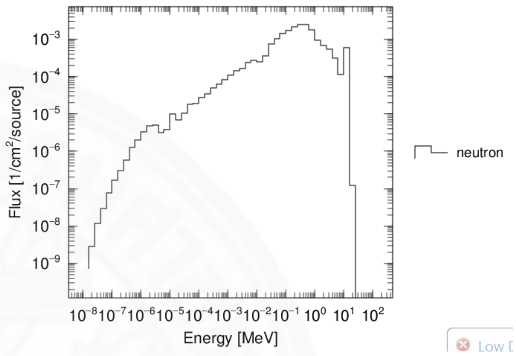
```
emin   = 1.e-8
emax   = 100.0                          $ MeV

part   =  neutron
unit   =  1                             $ (=1) 1/source, (=2) 1/cm^3/source
output =  source

axis   =  xy
file   =  source-xy.dat
gshow  =  3
epsout =  1
resol  =  1

[ T - Gshow ] off
    mesh =  xyz           # mesh type is xyz scoring mesh
  x-type =    2           # x-mesh is linear given by xmin, xmax and nx
      nx =   50           # number of x-mesh points
    xmin =  -150.         # minimum value of x-mesh points
    xmax =   150.         # maximum value of x-mesh points
  y-type =    2           # y-mesh is linear given by ymin, ymax and ny
      ny =   50           # number of y-mesh points
    ymin =  -150.         # minimum value of y-mesh points
    ymax =   150.         # maximum value of y-mesh points
  z-type =    1           # z-mesh is given by the below data
      nz =    1           # number of z-mesh points
          0.0  150.0
    axis =   xy           # axis of output
  output =    6           # (D=2) 1:bnd, 2:bnd+mat, 3:bnd+num 4:bnd+mat+num
    file = xy_gshow.dat    # file name of output for the above axis
   title = Check geometry using [T-gshow] tally
  epsout =    1           # (D=0) generate eps file by ANGEL

[ T - Gshow ] off
    mesh =  xyz           # mesh type is xyz scoring mesh
  x-type =    2           # x-mesh is linear given by xmin, xmax and nx
      nx =   50           # number of x-mesh points
    xmin =  -55.          # minimum value of x-mesh points
    xmax =   55.          # maximum value of x-mesh points
  y-type =    1           # y-mesh is given by the below data
      ny =    1           # number of y-mesh points
          -55.0  55.0
  z-type =    2           # z-mesh is linear given by zmin, zmax and nz
      nz =   50           # number of z-mesh points
    zmin =  -10.          # minimum value of z-mesh points
    zmax =   150.         # maximum value of z-mesh points
    axis =   xz           # axis of output
  output =    6           # (D=2) 1:bnd, 2:bnd+mat, 3:bnd+num 4:bnd+mat+num
```

```
    file = xz_gshow.dat    # file name of output for the above axis
   title = Check geometry using [T-gshow] tally
  epsout =    1           # (D=0) generate eps file by ANGEL
$
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
[end]
```

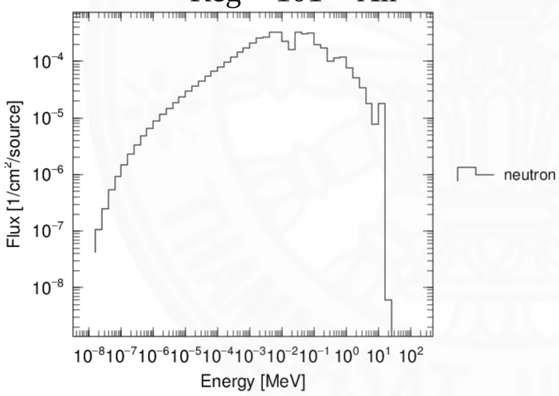
2.2. [T-Track] in region mesh



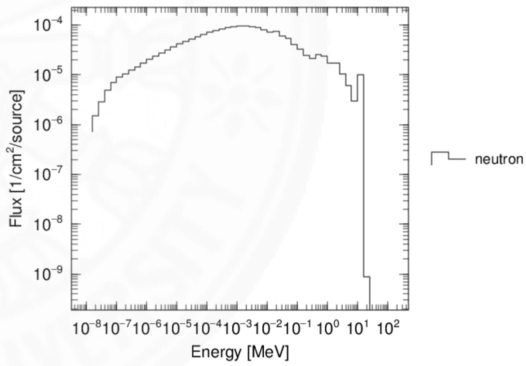
Reg = 101 = Air



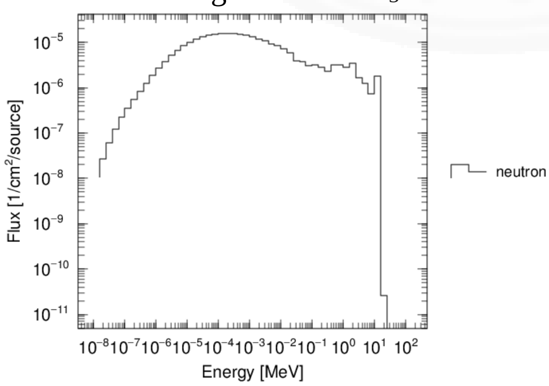
Reg = 102 = U



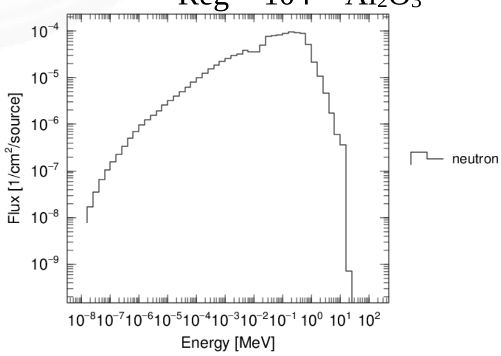
Reg = 103 = TiF_3



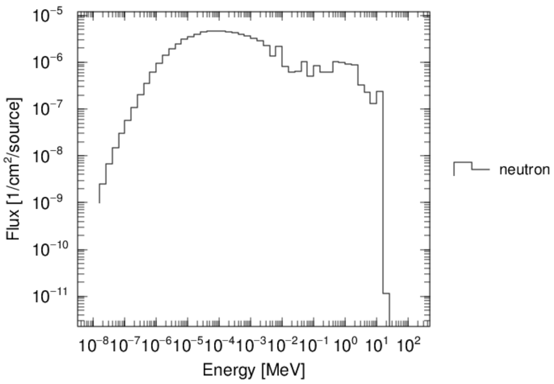
Reg = 104 = Al_2O_3



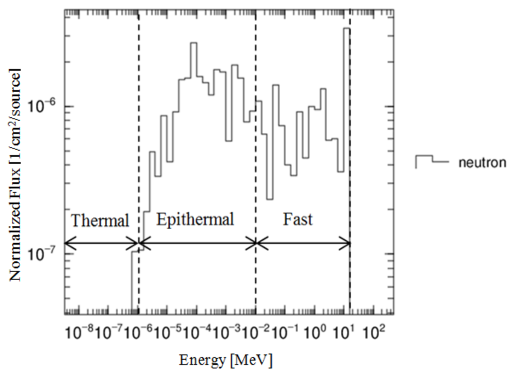
Reg = 105 = Ly-poly



Reg = 106 = Pb



Reg = 107 = Ni



Reg = 108 = Air

3. The BSA design proposed by Rasouli et al
3.1. input File
[title]
Example 1: Get started
$ "D" = default value
$ Comments with '$', '#', 'c'

$
%%%
%%%%%%%%%%
[parameters] $ Simulation parameters
file(6) = phits.out $ Output filename
maxcas   = 1e7 $ Number of events per batch
maxbch   = 1 $ Number of batch
imout   = 2 $ Option of material representation in [material] 2:MCNP-type
icntl   = 0 $ (D=0)Calculation mode: 0=real simulation, 5=no reactions (void all), 6=source check, 8=check geometry
itall   = 1 $ (D=0) Tally ouput after every batch. D=0 not output, D=1 output in same file

$ Cut-off energy
emin(1) = 1.0e-3 $ (D=1.0) cut-off energy for proton (MeV)
emin(2) = 1.e-10 $ (D=1.0) cut-off energy for neutron (MeV)
emin(12) = 1.e-1   # (D=1.d9) cut-off energy of electron (MeV)
emin(13) = 1.e-1   # (D=1.d9) cut-off energy of positron (MeV)
emin(14) = 1.e-3   # (D=1.d9) cut-off energy of photon (MeV)
emin(15) = 2.0e-3   # (D=1.d9) cut-off energy of deuteron (MeV/nucleon)
emin(16) = 3.0e-3   # (D=1.d9) cut-off energy of triton (MeV/nucleon)
emin(17) = 3.0e-3   # (D=1.d9) cut-off energy of 3He (MeV/nucleon)
emin(18) = 4.0e-3   # (D=1.d9) cut-off energy of Alpha (MeV/nucleon)
emin(19) = 1.0e-3   # (D=1.d9) cut-off energy of Heavy Ion (MeV/nucleon)

$ Maximum energy of nulcear data library used

$ By default, PHITS omits electron/positron/photon transport & uses Boltzmann transport for low-energy neutrons (<20MeV)
dmax(2) = 20.0 $ Neutron
dmax(12) = 1.0 $ Electron
dmax(13) = 1.0 $ positron
dmax(14) = 1.0 $ photon

$ Option for nuclear reactions
e-mode = 1 $ (D=0) Option for event-generator: 0=OFF, 1=ON
igamma = 1 $ (D=0) Option for gamma decay for residual nuclei: 0=no decay, 1=use 'trxcrd.dat', 2=EBITIM model, 3=EBITIM+isomer production
ipnint = 1 $ (D=0) Option for photonuclear reaction: 0=OFF, 1=ON
file(7) = data/xsdir.jnd $ Cross section data library for low energy neutrons
file(14)= data/trxcrd.dat $ Cross section data library for photon emission from residual nuclei

$ Option for charged particle transport
nedisp = 1 $ (D=0) Energy straggling: 0=OFF, 1=Landau-Vavilov
nspred = 2 $ (D=0) Angle straggling: 0=OFF, 2=Moliere First Coulomb diffusion
itstep = 1 $ (D=0) Option for timing tally "correct" curvature for momentum changing trajectory e.g. in magnetic field

$
%%%
%%%%%%%%%%
[source]
s-type = 1 % Source type: 1=cylinder, 2=rectangular, 9=spherical
proj = 2112 % Projectile: 2112=neutron
dir = 1 % Initial direction relative to positive-z axis: dir=cosine
e0 = 14.1 % Initial energy (MeV)

x0 = 0
y0 = 0
z0 = -1. % zmin (cm)
z1 = -1. % zmax: z1=z0 circle plan source
r0 = 1.7 % radius of the cylindrical source

$
%%%
%%%%%%%%%%
[material]
$ Material composition info: nuclei & density
$ Density can be defined in [cell], then in [material] you only need to define material compositions
$ i.e. weight fractions, if density is defined in g/cm^3, or atomic fractions if density in 10^24 atoms/cm^3

$ Library number and data class in "data/xsdir.jnd"

```
 MAT[1] $ Dry air, den=0.001205g/cc
         1001.50c              -0.125068
         1002.50c              -0.000287
         5010.50c              -0.018355
         5011.50c              -0.081645
         6000.50c              -0.774645

MAT[2] $ Uranium 238, den = 18.95g/cc
         92234.50c           -0.000057
          92235.50c         -0.007204
         92238.50c          -0.992739

MAT[3] $ Titanium trifluoride, den = 3.4 g/cc
         22048.50c           -0.336517056
             22046.50c       -0.037655035
             22049.50c       -0.024691003
             22047.50c       -0.033948418
             22050.50c       -0.023668488
             9019.50c        -0.54352

MAT[4] $ Fluental, den = 2.8232 gr/cc
        13027.50c            -0.3
        13027.50c          -0.2217
        9019.50c           -0.4683
        3006.50c           -0.0002
        3007.50c             -0.002475
        9019.50c             -0.007324

 MAT[5] $ Iron, den= 7.874 g/cc
       26054.50c            -0.0565
       26056.50c            -0.9190
       26057.50c            -0.0216
       26058.50c            -0.0029

 MAT[6] $ Lithium, den = 0.534 g/cc
       3006.50c          -0.075
       3007.50c           -0.925

 MAT[7] $ bismuth, den = 9.747 g/cc
       83209.50c          -1.0000

MAT[8] $ Lead, den = 11.35 g/cc
      82204.50c           -0.01378
      82206.50c           -0.23955
      82207.50c           -0.22074
```

```
      82208.50c          -0.52592

 MAT[9] $ Lithium Fluoride, den = 2.635  g/cc
      3006.50c        -0.020069
      3007.50c        -0.247516
      9019.50c        -0.732415

 MAT[10] $ Dry air, den=0.001205g/cc
      1001.50c           -0.125068
      1002.50c           -0.000287
      5010.50c           -0.018355
      5011.50c           -0.081645
      6000.50c           -0.774645

 $
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
 [mat name color]
 mat    name          size    color
 0        void          1       white
 1     air              1     blue
 2        U             1       violet
 3     TiF3             1     red
 4     Fluental         1     bluegreen
 5     Fe               1     mossgreen
 6     Li               1     yellow
 7     Bi               1     pastelpink
 8     Pb               1     pastelbrown
 9     LiF              1     darkgray
 10     air              1      cyan

$
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
[ S u r f a c e ]
  10  so      500.
  11  cz      1.7                              $ air(1)
  12  pz      0.                               $
  13  pz      63.                              $
  14  sph      0 0 63 14                        $ U (2)
  15  cz      36.                              $ TiF3 (3)
  16  pz      63.                               $
  17  pz      86.                               $
  18  TRC      0. 0. 0. 0. 0. 36.  36.  12.       $ Fluental (4)
  19  TRC      0. 0. 0. 0. 0. 4.   12.  10.       $ Fe (5)
  20  TRC      0. 0. 0. 0. 0. 2.   10.  8.        $ Li (6)
  21  TRC      0. 0. 0. 0. 0. 3.   8.    6.       $ Bi (7)
```

```
  22  cz      38.                              $ Pb (8)
  23  pz      0.                               $
  24  pz      86.                        $
  25  cz      38.                        $ LiF (9)
  26  pz      86.                        $
  27  pz      131.                       $
  28  sph      0. 0. 0. 1.               $ air (10), detecor

$
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
[cell]
$ If density is positive: unit 10^24 atoms/cm^3 (= atoms/barn/cm)
$ If density is negative: unit g/cm^3

$id    mat    den            surface
  100   -1      10
  101   1       -0.001205     -11  12  -13
  102   2       -18.95        -14              #101
  103   3       -3.4          -15  16  -17      #101 #102
  104   4       -2.8232       -18               trcl=(0 0 86)
  105   5       -7.874        -19              trcl=(0 0 122)
  106   6       -0.534        -20               trcl=(0 0 126)
  107   7       -9.747        -21               trcl=(0 0 128)
  108   8       -11.35        -22 23 -24        #101 #102 #103
  109    9         -2.635        -25 26 -27        #104 #105 #106 #107 #108
  110   10      -0.001205     -28              trcl=(0 0 132)
  111   0       -10                         #101  #102 #103  #104 #105  #106 #107 #108 #109
#110           $ working area

$
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
[volume]
reg              vol
101              571.69          $ cell 1
102           11361.168
103           87853.013
104           70536.96
105           1523.95
106           510.773
107           464.72
108           208042.97
109           131000.797
110           4.19
```

```
$
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%
[ T - product ]off        $ Check product-eng

mesh    = reg
reg     = {101-105}

e-type  = 3                           $ (=3) log scale
ne      = 50
emin    = 1.e-8
emax    = 100.                        $ MeV

mother  = all

part    = Neutron Photon
unit    = 1                           $ 1/source

axis   =  eng
file   =  product-eng.dat
gshow  =  3
epsout =  1
resol  =  1

[t-track] off             $xy: check geometry
$Region crossing tally

mesh   = xyz

z-type = 1
nz     = 3
          -5 0 10 20 30 45

x-type = 2
nx     = 100
xmin   = -15
xmax   = 15

y-type = 2
ny     = 100
ymin   = -15
ymax   = 15

e-type = 3                            $ All energies
ne     = 1
emin   = 1e-8
emax   = 1e2                          $ MeV
```

part   = Neutron Photon $ 2112=neutron 22=photon
unit   = 1 $ 1/cm^2/source

axis   = xy
file   = track-xy.dat $ all particles in one diagram
gshow = 3 $ 2: region boundary & material name; 3: region
boundary and name
epsout = 1
resol = 1

$
%%
%%%%%%%%%%%
[t-track]off $yz: check geometry
$Region crossing tally

mesh   = xyz

x-type = 1
nx   = 3
            -5 -0 +30 +50

y-type = 2
ny   = 100
ymin   = -50
ymax   = 50

z-type = 2
nz   = 100
zmin   = -5
zmax   = 100

e-type = 3 $ All energies
ne   = 1
emin   = 1e-8
emax   = 1e2 $ MeV

part   = Neutron $ 2112=neutron 22=photon
unit   = 1 $ 1/cm^2/source

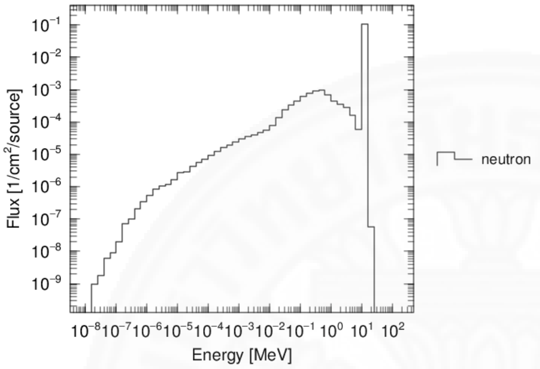
axis   = yz
file   = track-yz.dat $ all particles in one diagram
gshow = 3 $ 2: region boundary & material name; 3: region
boundary and region name
epsout = 1
resol = 1

```
$
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%
[T-track]                        $ Tally particle energies in detectors
$ Region crossing tally

mesh    = reg
reg     = {101-110}
e-type  = 3                             $ (=3) log scale
ne      = 50
emin    = 1.e-8
emax    = 100.                          $ MeV

part    = Neutron                $ 2112=neutron, 22=photon, 2212=proton
unit    = 1                             $ 1/cm^2/source

axis    = eng
file    = track-reg-eng-26e7.dat                $ all particles in one diagram
gshow   = 3                             $ 2: region boundary & material name; 3: region
boundary and name
epsout  = 1
resol   = 1

$
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%
[ T - product ]  off      $ Check source xy

mesh   = xyz

z-type = 1
nz     = 3
         -5 0 10 20 30 45

x-type = 2
nx     = 100
xmin   = -30
xmax   = 30

y-type = 2
ny     = 100
ymin   = -30
ymax   = 30

e-type = 3                              $ All energies
ne     = 1
```

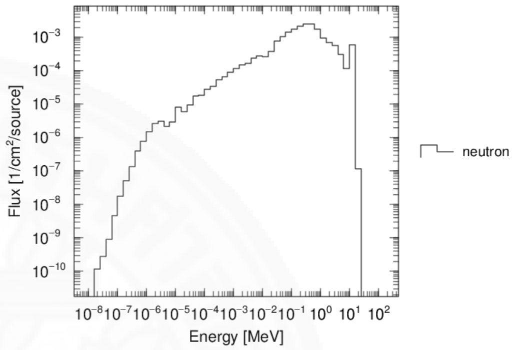
```
emin   = 1.e-8
emax   = 100.0                              $ MeV

part   =  neutron
unit   =  1                                 $ (=1) 1/source, (=2) 1/cm^3/source
output =  source

axis   =  xy
file   =  source-xy.dat
gshow  =  3
epsout =  1
resol  =  1

[ T - Gshow ]  off
     mesh =  xyz           # mesh type is xyz scoring mesh
   x-type =    2           # x-mesh is linear given by xmin, xmax and nx
       nx =   50           # number of x-mesh points
     xmin =  -50.          # minimum value of x-mesh points
     xmax =   50.          # maximum value of x-mesh points
   y-type =    2           # y-mesh is linear given by ymin, ymax and ny
       ny =   50           # number of y-mesh points
     ymin =  -50.          # minimum value of y-mesh points
     ymax =   50.          # maximum value of y-mesh points
   z-type =    1           # z-mesh is given by the below data
       nz =    1           # number of z-mesh points
           0.0  45.0
     axis =   xy           # axis of output
   output =    6           # (D=2) 1:bnd, 2:bnd+mat, 3:bnd+num 4:bnd+mat+num
     file = xy_gshow.dat    # file name of output for the above axis
    title = Check geometry using [T-gshow] tally
   epsout =    1           # (D=0) generate eps file by ANGEL

[ T - Gshow ] off
     mesh =  xyz           # mesh type is xyz scoring mesh
   x-type =    2           # x-mesh is linear given by xmin, xmax and nx
       nx =   50           # number of x-mesh points
     xmin =  -55.          # minimum value of x-mesh points
     xmax =   55.          # maximum value of x-mesh points
   y-type =    1           # y-mesh is given by the below data
       ny =    1           # number of y-mesh points
          -55.0  55.0
   z-type =    2           # z-mesh is linear given by zmin, zmax and nz
       nz =   50           # number of z-mesh points
     zmin =  -10.          # minimum value of z-mesh points
     zmax =   150.         # maximum value of z-mesh points
     axis =   xz           # axis of output
   output =    6           # (D=2) 1:bnd, 2:bnd+mat, 3:bnd+num 4:bnd+mat+num
```

file = xz_gshow.dat   # file name of output for the above axis
title = Check geometry using [T-gshow] tally
epsout =   1   # (D=0) generate eps file by ANGEL
$
%%%
%%%%%%%%%%%
[end]

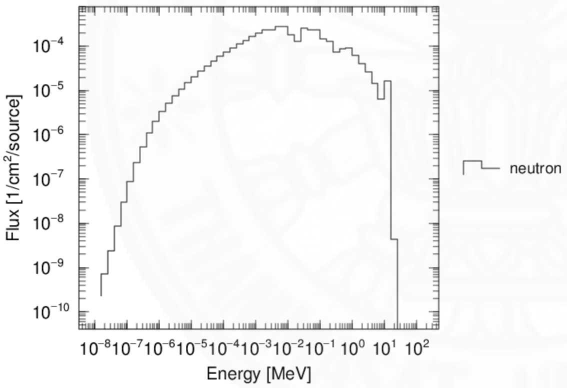
3.2. . [T-Track] in region mesh



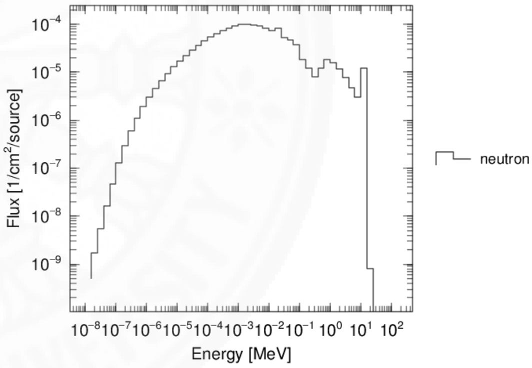
Reg = 101 = Air



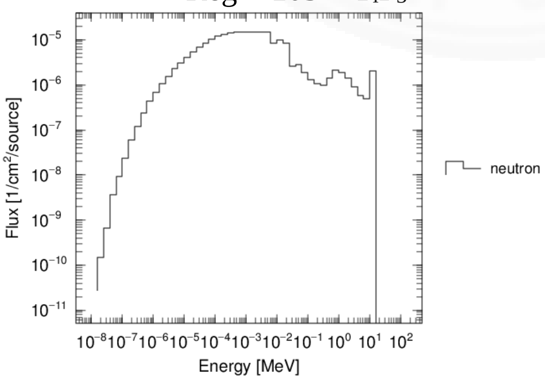
Reg = 102 = U



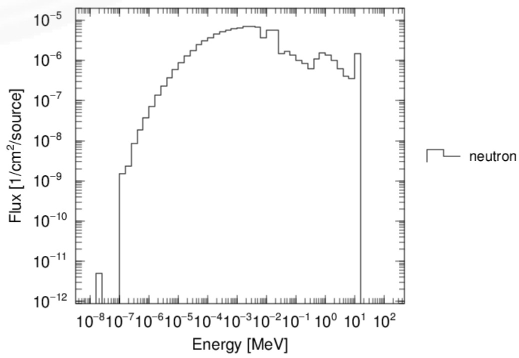
Reg = 103 = T_iF_3



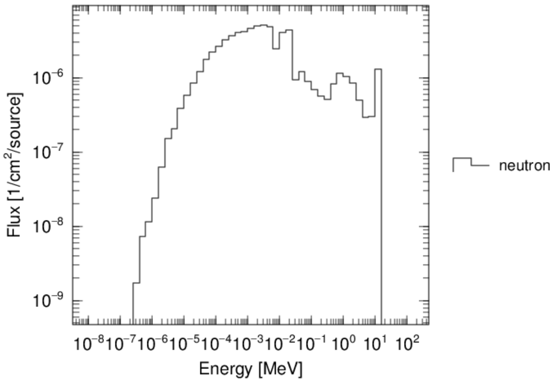
Reg = 104 = Fluental



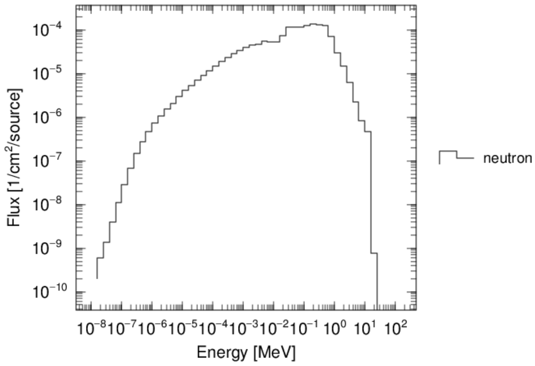
Reg = 105 = Fe



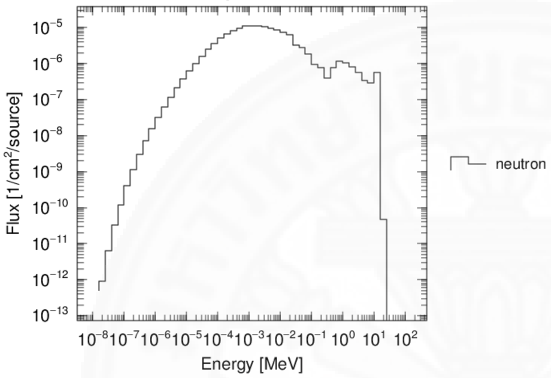
Reg = 106 = Li



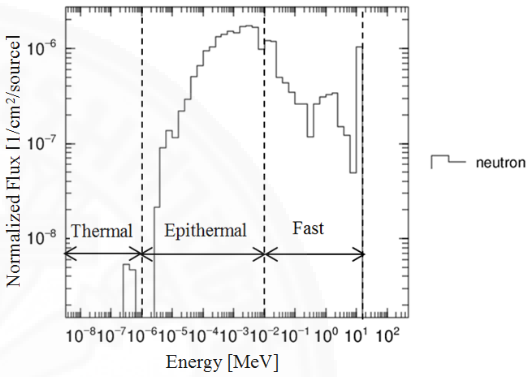
Reg = 107 = Bi



Reg = 108 = Pb



Reg = 109 = LiF



Reg = 110 = Air

Appendix B

Development of BSA

1. Pb as a Multiplier
1.1. Input file

```
[title]
Example 1: Get started
$ "D" = default value
$ Comments with '$', '#', 'c'

$
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%
[parameters]          $ Simulation parameters
file(6)  = phits.out  $ Output filename
maxcas   = 1e7              $ Number of events per batch
maxbch   = 1          $ Number of batch
imout    = 2          $ Option of material representation in [material] 2:MCNP-type
icntl    = 0           $ (D=0)Calculation mode: 0=real simulation, 5=no reactions
(void all), 6=source check, 8=check geometry
itall    = 1          $ (D=0) Tally ouput after every batch. D=0 not output, D=1
output in same file

$ Cut-off energy
emin(1)  = 1.0e-3     $ (D=1.0) cut-off energy for proton (MeV)
emin(2)  = 1.e-10     $ (D=1.0) cut-off energy for neutron (MeV)
emin(12) = 1.e-1      # (D=1.d9) cut-off energy of electron (MeV)
emin(13) = 1.e-1      # (D=1.d9) cut-off energy of positron (MeV)
emin(14) = 1.e-3      # (D=1.d9) cut-off energy of photon (MeV)
emin(15) = 2.0e-3     # (D=1.d9) cut-off energy of deuteron (MeV/nucleon)
emin(16) = 3.0e-3     # (D=1.d9) cut-off energy of triton (MeV/nucleon)
emin(17) = 3.0e-3     # (D=1.d9) cut-off energy of 3He (MeV/nucleon)
emin(18) = 4.0e-3     # (D=1.d9) cut-off energy of Alpha (MeV/nucleon)
emin(19) = 1.0e-3     # (D=1.d9) cut-off energy of Heavy Ion (MeV/nucleon)

$ Maximum energy of nulcear data library used
$ By default, PHITS omits electron/positron/photon transport & uses Boltzmann
transport for low-energy neutrons (<20MeV)
dmax(2)  = 20.0             $ Neutron
dmax(12) = 1.0              $ Electron
dmax(13) = 1.0              $ positron
dmax(14) = 1.0              $ photon

$ Option for nuclear reactions
```

e-mode = 1 $ (D=0) Option for event-generator: 0=OFF, 1=ON
igamma = 1 $ (D=0) Option for gamma decay for residual nuclei: 0=no decay, 1=use 'trxcrd.dat', 2=EBITIM model, 3=EBITIM+isomer production
ipnint = 1 $ (D=0) Option for photonuclear reaction: 0=OFF, 1=ON
file(7) = data/xsdir.jnd $ Cross section data library for low energy neutrons
file(14)= data/trxcrd.dat $ Cross section data library for photon emission from residual nuclei

$ Option for charged particle transport
nedisp   = 1 $ (D=0) Energy straggling: 0=OFF, 1=Landau-Vavilov
nspred   = 2 $ (D=0) Angle straggling: 0=OFF, 2=Moliere First Coulomb diffusion
itstep   = 1 $ (D=0) Option for timing tally "correct" curvature for momentum changing trajectory e.g. in magnetic field

$
%%
%%%%%%%%%%%%%%%%%%%%
[source]
s-type = 1   % Source type: 1=cylinder, 2=rectangular, 9=spherical
proj   = 2112   % Projectile: 2112=neutron
dir   = 1   % Initial direction relative to positive-z axis: dir=cosine
e0   = 2.45   % Initial energy (MeV)

x0   = 0
y0   = 0
z0   = 0.   % zmin (cm)
z1   = 0.   % zmax: z1=z0 circle plan source
r0   = 1.7   % radius of the cylindrical source

$
%%
%%%%%%%%%%%%%%%%%%%%
[material]
$ Material composition info: nuclei & density
$ Density can be defined in [cell], then in [material] you only need to define material compositions
$ i.e. weight fractions, if density is defined in g/cm^3, or atomic fractions if density in 10^24 atoms/cm^3
$ Library number and data class in "data/xsdir.jnd"

  MAT[1] $ Lead, den = 11.35 g/cc
          82204.50c   -0.01378
          82206.50c   -0.23955
          82207.50c   -0.22074
          82208.50c   -0.52592

```
 MAT[2] $ Dry air, den=0.001205g/cc
            6000.50c        -0.000124
            7014.50c        -0.752291
            7015.50c        -0.002977
            8016.50c        -0.231781
           18040.50c        -0.012827

 $
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
 [mat name color]
 mat     name              size      color
 0         void              1          white
 1         Pb                  1          camel
 2          air                 1          blue

$
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
[ S u r f a c e ]
  10  so     500.
  11  cz       20.                        $ 20 cm radius of Pb and 4 cm thickness
  12  pz       0.
  13  pz       4.
  14  sph     0 0 0 1              $ Air 1 cm radius, detector

$
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
[cell]
$ If density is positive: unit 10^24 atoms/cm^3 (= atoms/barn/cm)
$ If density is negative: unit g/cm^3

$id     mat     den              surface
 100    -1       10
  101   1       -11.35         -11  12  -13
  102   2       -0.001205    -14                     trcl=(0 0 5)
  110   0                         -10   #101  #102                          $ working area

 $
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
 [volume]
 reg               vol
 101               5024.             $ cell 1
 102             4.19
```

```
$
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%
[ T - product ]off        $ Check product-eng

mesh    = reg
reg     = {101-105}

e-type  = 3                           $ (=3) log scale
ne      = 50
emin    = 1.e-8
emax    = 100.                        $ MeV

mother  = all

part    = Neutron Photon
unit    = 1                           $ 1/source

axis   =  eng
file   =  product-eng.dat
gshow  =  3
epsout =  1
resol  =  1

[t-track] off             $xy: check geometry
$Region crossing tally

mesh   = xyz

z-type = 1
nz     = 3
           -5 0 10 20 30 45

x-type = 2
nx     = 100
xmin   = -15
xmax   = 15

y-type = 2
ny     = 100
ymin   = -15
ymax   = 15

e-type = 3                            $ All energies
ne     = 1
emin   = 1e-8
emax   = 1e2                          $ MeV
```

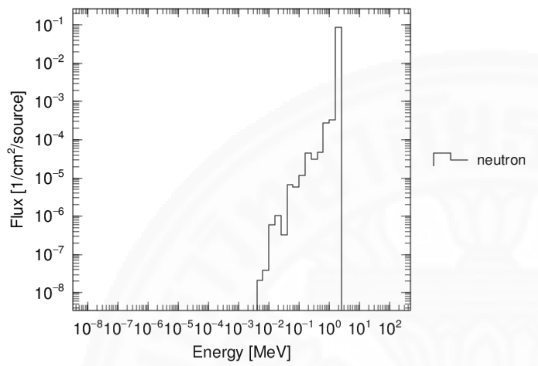
```
part   = Neutron Photon                         $ 2112=neutron 22=photon
unit   = 1                              $ 1/cm^2/source

axis   = xy
file   = track-xy.dat                   $ all particles in one diagram
gshow  = 3                              $ 2: region boundary & material name; 3: region
boundary and name
epsout = 1
resol  = 1

$
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%
[t-track] off              $yz: check geometry
$Region crossing tally

mesh   = xyz

x-type = 1
nx     = 3
            -30 -10 +10 +30

y-type = 2
ny     = 100
ymin   = -30
ymax   = 30

z-type = 2
nz     = 100
zmin   = -5
zmax   = 60

e-type = 3                              $ All energies
ne     = 1
emin   = 1e-8
emax   = 1e2                            $ MeV

part   = Neutron Photon                         $ 2112=neutron 22=photon
unit   = 1                              $ 1/cm^2/source

axis   = yz
file   = track-yz.dat                   $ all particles in one diagram
gshow  = 3                              $ 2: region boundary & material name; 3: region
boundary and region name
epsout = 1
resol  = 1
```

```
$
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%
[T-track]                    $ Tally particle energies in detectors
$ Region crossing tally

mesh    = reg
reg     = {101-102}
e-type  = 3                          $ (=3) log scale
ne      = 50
emin    = 1.e-8
emax    = 100.                       $ MeV

part    = Neutron            $ 2112=neutron, 22=photon, 2212=proton
unit    = 1                          $ 1/cm^2/source

axis    = eng
file    = track-reg-eng-DDMul4.dat           $ all particles in one diagram
gshow   = 3                          $ 2: region boundary & material name; 3: region
boundary and name
epsout  = 1
resol   = 1

$
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%
[ T - product ]  off      $ Check source xy

mesh   = xyz

z-type = 1
nz     = 3
         -5 0 10 20 30 45

x-type = 2
nx     = 100
xmin   = -30
xmax   = 30

y-type = 2
ny     = 100
ymin   = -30
ymax   = 30

e-type = 3                           $ All energies
ne     = 1
```

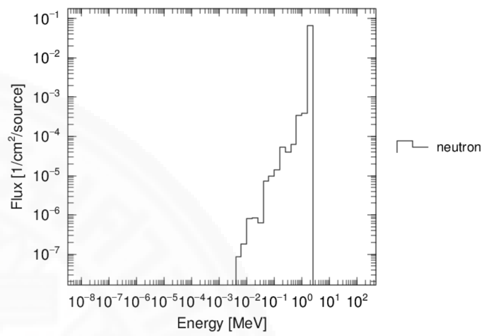
```
emin   = 1.e-8
emax   = 100.0                          $ MeV

part   =  neutron
unit   =  1                             $ (=1) 1/source, (=2) 1/cm^3/source
output =  source

axis   =  xy
file   =  source-xy.dat
gshow  =  3
epsout =  1
resol  =  1

[ T - Gshow ] off
    mesh =  xyz          # mesh type is xyz scoring mesh
  x-type =    2          # x-mesh is linear given by xmin, xmax and nx
      nx =   50          # number of x-mesh points
    xmin =  -25.         # minimum value of x-mesh points
    xmax =   25.         # maximum value of x-mesh points
  y-type =    2          # y-mesh is linear given by ymin, ymax and ny
      ny =   50          # number of y-mesh points
    ymin =  -25.         # minimum value of y-mesh points
    ymax =   25.         # maximum value of y-mesh points
  z-type =    1          # z-mesh is given by the below data
      nz =    1          # number of z-mesh points
         0.0  25.0
    axis =   xy          # axis of output
  output =    6          # (D=2) 1:bnd, 2:bnd+mat, 3:bnd+num 4:bnd+mat+num
    file = xy_gshow.dat    # file name of output for the above axis
   title = Check geometry using [T-gshow] tally
  epsout =    1          # (D=0) generate eps file by ANGEL

[ T - Gshow ] off
    mesh =  xyz          # mesh type is xyz scoring mesh
  x-type =    2          # x-mesh is linear given by xmin, xmax and nx
      nx =   50          # number of x-mesh points
    xmin =  -25.         # minimum value of x-mesh points
    xmax =   25.         # maximum value of x-mesh points
  y-type =    1          # y-mesh is given by the below data
      ny =    1          # number of y-mesh points
         -25.0  25.0
  z-type =    2          # z-mesh is linear given by zmin, zmax and nz
      nz =   50          # number of z-mesh points
    zmin =  -10.         # minimum value of z-mesh points
    zmax =   80.         # maximum value of z-mesh points
    axis =   xz          # axis of output
  output =    6          # (D=2) 1:bnd, 2:bnd+mat, 3:bnd+num 4:bnd+mat+num
```

file = xz_gshow.dat   # file name of output for the above axis
title = Check geometry using [T-gshow] tally
epsout =   1   # (D=0) generate eps file by ANGEL
$
%%
%%%%%%%%%%%
[end]

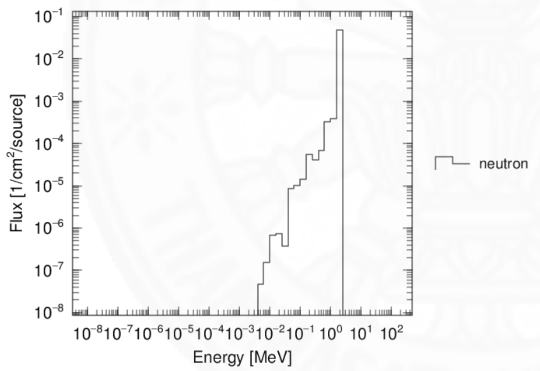
1.2. T-Track



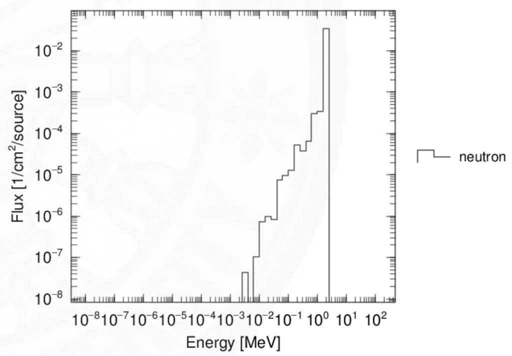
2 cm



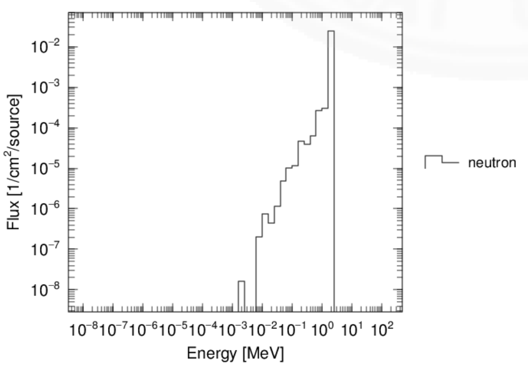
4 cm



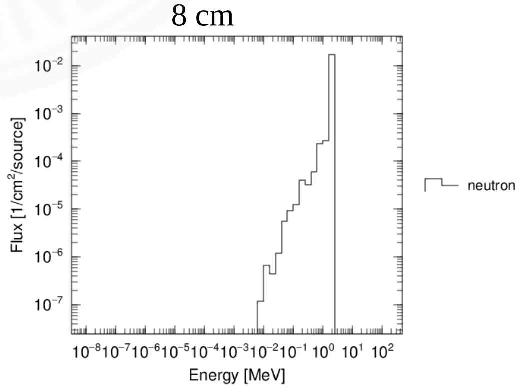
6 cm



8 cm



10 cm



12 cm

2. TiF_3 as the first moderator
2.1 input file

```
[title]
Example 1: Get started
$ "D" = default value
$ Comments with '$', '#', 'c'

$
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%
[parameters]             $ Simulation parameters
file(6)  = phits.out     $ Output filename
maxcas   = 1e7                   $ Number of events per batch
maxbch   = 1             $ Number of batch
imout    = 2             $ Option of material representation in [material] 2:MCNP-type
icntl    = 0             $ (D=0)Calculation mode: 0=real simulation, 5=no reactions
(void all), 6=source check, 8=check geometry
itall    = 1             $ (D=0) Tally ouput after every batch. D=0 not output, D=1
output in same file

$ Cut-off energy
emin(1)  = 1.0e-3        $ (D=1.0) cut-off energy for proton (MeV)
emin(2)  = 1.e-10        $ (D=1.0) cut-off energy for neutron (MeV)
emin(12) = 1.e-1         # (D=1.d9) cut-off energy of electron (MeV)
emin(13) = 1.e-1         # (D=1.d9) cut-off energy of positron (MeV)
emin(14) = 1.e-3         # (D=1.d9) cut-off energy of photon (MeV)
emin(15) = 2.0e-3        # (D=1.d9) cut-off energy of deuteron (MeV/nucleon)
emin(16) = 3.0e-3        # (D=1.d9) cut-off energy of triton (MeV/nucleon)
emin(17) = 3.0e-3        # (D=1.d9) cut-off energy of 3He (MeV/nucleon)
emin(18) = 4.0e-3        # (D=1.d9) cut-off energy of Alpha (MeV/nucleon)
emin(19) = 1.0e-3        # (D=1.d9) cut-off energy of Heavy Ion (MeV/nucleon)

$ Maximum energy of nulcear data library used
$ By default, PHITS omits electron/positron/photon transport & uses Boltzmann
transport for low-energy neutrons (<20MeV)
dmax(2)  = 20.0                  $ Neutron
dmax(12) = 1.0                   $ Electron
dmax(13) = 1.0                   $ positron
dmax(14) = 1.0                   $ photon

$ Option for nuclear reactions
e-mode  = 1              $ (D=0) Option for event-generator: 0=OFF, 1=ON
igamma  = 1              $ (D=0) Option for gamma decay for residual nuclei: 0=no
decay, 1=use 'trxcrd.dat', 2=EBITIM model, 3=EBITIM+isomer production
ipnint  = 1      $ (D=0) Option for photonuclear reaction: 0=OFF, 1=ON
file(7) = data/xsdir.jnd         $ Cross section data library for low energy neutrons
file(14)= data/trxcrd.dat        $ Cross section data library for photon emission from
residual nuclei
```

```
$ Option for charged particle transport
nedisp   = 1                $ (D=0) Energy straggling: 0=OFF, 1=Landau-Vavilov
nspred   = 2                $ (D=0) Angle straggling: 0=OFF, 2=Moliere First Coulomb
diffusion
itstep   = 1                $ (D=0) Option for timing tally "correct" curvature for
momentum changing trajectory e.g. in magnetic field

$
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%
[source]
s-type  = 1                 % Source type: 1=cylinder, 2=rectangular, 9=spherical
proj     = 2112             % Projectile: 2112=neutron
dir      = 1                % Initial direction relative to positive-z axis: dir=cosine
e0       = 2.45             % Initial energy (MeV)

x0     = 0
y0     = 0
z0       = 0.               % zmin (cm)
z1       = 0.               % zmax:  z1=z0 circle plan source
r0       = 1.7              % radius of the cylindrical source

$
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%
[material]
$ Material composition info: nuclei & density
$ Density can be defined in [cell], then in [material] you only need to define material
compositions
$ i.e. weight fractions, if density is defined in g/cm^3, or atomic fractions if density in
10^24 atoms/cm^3
$ Library number and data class in "data/xsdir.jnd"

  MAT[1] $ Lead, den = 11.35 g/cc
          82204.50c         -0.01378
          82206.50c         -0.23955
          82207.50c         -0.22074
          82208.50c         -0.52592

 MAT[2] $ Titanium trifluoride, den = 3.4 g/cc
            22048.50c         -0.336517056
            22046.50c         -0.037655035
            22049.50c         -0.024691003
            22047.50c         -0.033948418
            22050.50c         -0.023668488
            9019.50c          -0.54352
```

```
 MAT[3] $ Dry air, den=0.001205g/cc
            6000.50c       -0.000124
            7014.50c       -0.752291
            7015.50c       -0.002977
            8016.50c       -0.231781
            18040.50c      -0.012827

 $
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%
 [mat name color]
 mat    name            size    color
 0      void            1       white
 1      Pb              1       camel
 2      TiF3            1       pink
 3    air               1       blue

$
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%
[ S u r f a c e ]
  10  so     500.
  11  cz      20.              $ 20 cm radius of Pb and 4 cm thickness
  12  pz      0.
  13  pz      4.
  14  cz      20.              $ 20 cm radius of Tif3 and 16 cm thickness
  15  pz      4.
  16  pz      20.
  17  sph     0 0 0 1          $ Air 1 cm radius, detector

$
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%
[cell]
$ If density is positive: unit 10^24 atoms/cm^3 (= atoms/barn/cm)
$ If density is negative: unit g/cm^3

$id    mat    den           surface
 100   -1     10
  101  1      -11.35      -11  12  -13
  102  2      -3.4        -14  15  -16
  103  3         -0.001205    -17                 trcl=(0 0 21)
  110  0      -10   #101  #102  #103                      $ working area

 $
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%
```

```
[volume]
reg             vol
101             5024.           $ cell 1
102             20096.
103             4.19

$
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%
[ T - product ]off       $ Check product-eng

mesh    = reg
reg     = {101-105}

e-type  = 3                         $ (=3) log scale
ne      = 50
emin    = 1.e-8
emax    = 100.                      $ MeV

mother  = all

part    = Neutron Photon
unit    = 1                         $ 1/source

axis   =  eng
file   =  product-eng.dat
gshow  =  3
epsout =  1
resol  =  1

[t-track] off            $xy: check geometry
$Region crossing tally

mesh   = xyz

z-type = 1
nz     = 3
         -5 0 10 20 30 45

x-type = 2
nx     = 100
xmin   = -15
xmax   = 15

y-type = 2
ny     = 100
ymin   = -15
```

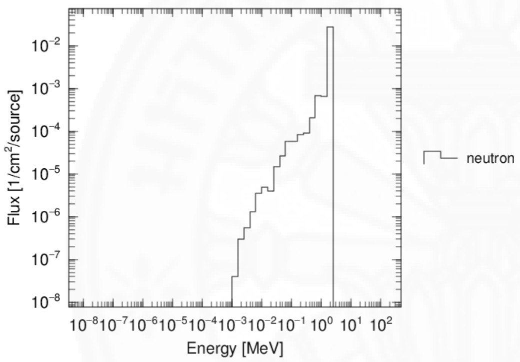
```
ymax   = 15

e-type = 3                          $ All energies
ne     = 1
emin   = 1e-8
emax   = 1e2                        $ MeV

part   = Neutron Photon                     $ 2112=neutron 22=photon
unit   = 1                          $ 1/cm^2/source

axis   = xy
file   = track-xy.dat               $ all particles in one diagram
gshow  = 3                          $ 2: region boundary & material name; 3: region
boundary and name
epsout = 1
resol  = 1

$
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%
[t-track] off             $yz: check geometry
$Region crossing tally

mesh   = xyz

x-type = 1
nx     = 3
          -30 -10 +10 +30

y-type = 2
ny     = 100
ymin   = -30
ymax   = 30

z-type = 2
nz     = 100
zmin   = -5
zmax   = 60

e-type = 3                          $ All energies
ne     = 1
emin   = 1e-8
emax   = 1e2                        $ MeV

part   = Neutron Photon                     $ 2112=neutron 22=photon
unit   = 1                          $ 1/cm^2/source
```

```
axis   = yz
file   = track-yz.dat                    $ all particles in one diagram
gshow  = 3                               $ 2: region boundary & material name; 3: region
boundary and region name
epsout = 1
resol  = 1

$
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%
[T-track]                        $ Tally particle energies in detectors
$ Region crossing tally

mesh    = reg
reg     = {101-103}
e-type  = 3                              $ (=3) log scale
ne      = 50
emin    = 1.e-8
emax    = 100.                           $ MeV

part    = Neutron                $ 2112=neutron, 22=photon, 2212=proton
unit    = 1                              $ 1/cm^2/source

axis    = eng
file    = track-reg-eng-DDmode16.dat                 $ all particles in one diagram
gshow   = 3                              $ 2: region boundary & material name; 3: region
boundary and name
epsout  = 1
resol   = 1

$
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%
[ T - product ]  off       $ Check source xy

mesh   = xyz

z-type = 1
nz     = 3
          -5 0 10 20 30 45

x-type = 2
nx     = 100
xmin   = -30
xmax   = 30

y-type = 2
```

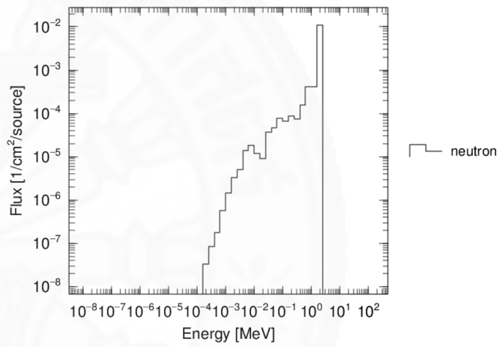
```
ny     = 100
ymin   = -30
ymax   = 30

e-type = 3                              $ All energies
ne     = 1
emin   = 1.e-8
emax   = 100.0                          $ MeV

part   =  neutron
unit   =  1                             $ (=1) 1/source, (=2) 1/cm^3/source
output =  source

axis   =  xy
file   =  source-xy.dat
gshow  =  3
epsout =  1
resol  =  1

[ T - Gshow ] off
    mesh =  xyz           # mesh type is xyz scoring mesh
  x-type =    2           # x-mesh is linear given by xmin, xmax and nx
      nx =   50           # number of x-mesh points
    xmin =  -25.          # minimum value of x-mesh points
    xmax =   25.          # maximum value of x-mesh points
  y-type =    2           # y-mesh is linear given by ymin, ymax and ny
      ny =   50           # number of y-mesh points
    ymin =  -25.          # minimum value of y-mesh points
    ymax =   25.          # maximum value of y-mesh points
  z-type =    1           # z-mesh is given by the below data
      nz =    1           # number of z-mesh points
         0.0  25.0
    axis =   xy           # axis of output
  output =    6           # (D=2) 1:bnd, 2:bnd+mat, 3:bnd+num 4:bnd+mat+num
    file = xy_gshow.dat    # file name of output for the above axis
   title = Check geometry using [T-gshow] tally
  epsout =    1           # (D=0) generate eps file by ANGEL

[ T - Gshow ] off
    mesh =  xyz           # mesh type is xyz scoring mesh
  x-type =    2           # x-mesh is linear given by xmin, xmax and nx
      nx =   50           # number of x-mesh points
    xmin =  -25.          # minimum value of x-mesh points
    xmax =   25.          # maximum value of x-mesh points
  y-type =    1           # y-mesh is given by the below data
      ny =    1           # number of y-mesh points
         -25.0  25.0
```

```
  z-type =    2           # z-mesh is linear given by zmin, zmax and nz
      nz =   50           # number of z-mesh points
    zmin =  -10.          # minimum value of z-mesh points
    zmax =   80.          # maximum value of z-mesh points
    axis =   xz           # axis of output
  output =    6           # (D=2) 1:bnd, 2:bnd+mat, 3:bnd+num 4:bnd+mat+num
    file = xz_gshow.dat    # file name of output for the above axis
   title = Check geometry using [T-gshow] tally
  epsout =    1           # (D=0) generate eps file by ANGEL
$
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
[end]
```

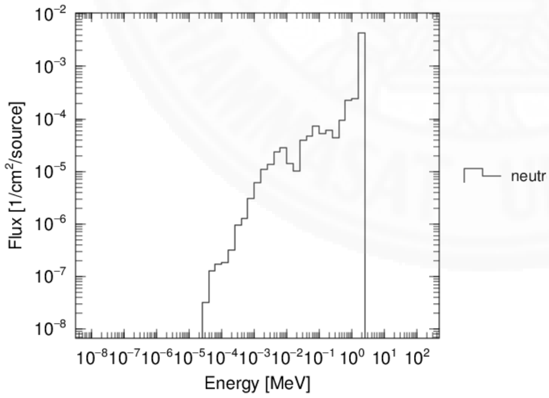
2.2. [t-track]



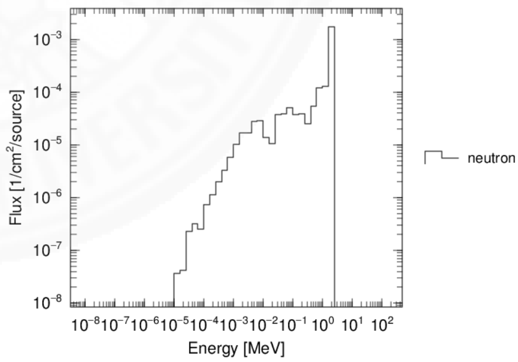
4 cm



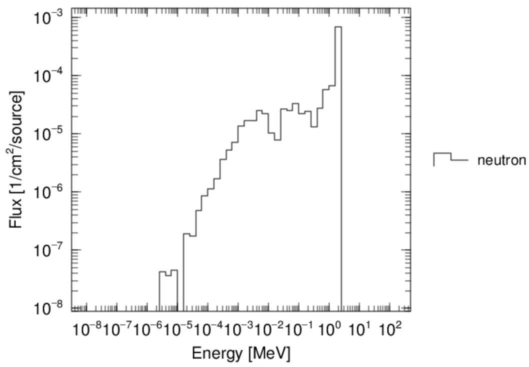
8 cm



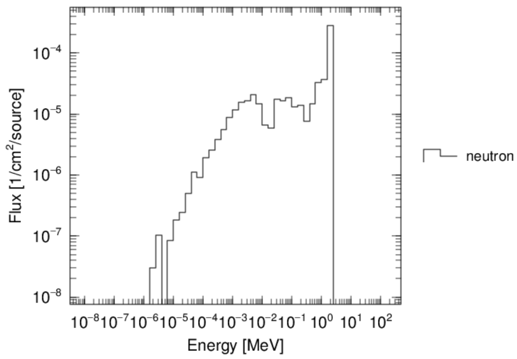
12 cm



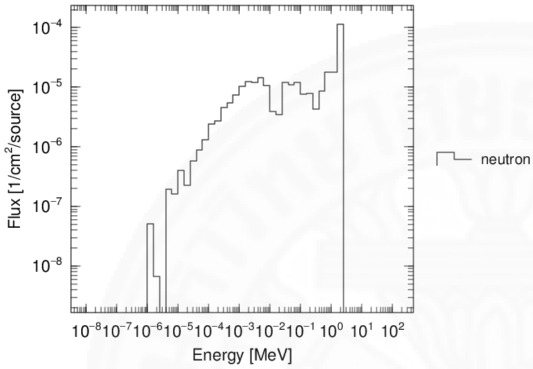
16 cm



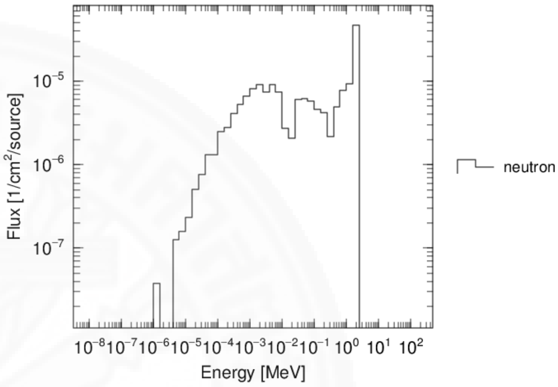
20 cm



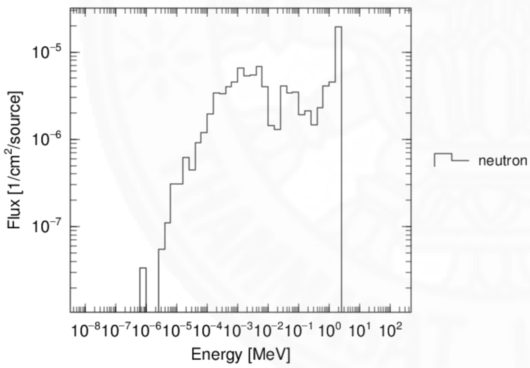
24 cm



28 cm



32 cm



36 cm

3. AlF3 as the second moderator
3.1. input file

```
[title]
Example 1: Get started
$ "D" = default value
$ Comments with '$', '#', 'c'

$
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
[parameters]            $ Simulation parameters
file(6)  = phits.out    $ Output filename
```

maxcas = 1e7 $ Number of events per batch
maxbch = 1 $ Number of batch
imout = 2 $ Option of material representation in [material] 2:MCNP-type
icntl = 0 $ (D=0)Calculation mode: 0=real simulation, 5=no reactions (void all), 6=source check, 8=check geometry
itall = 1 $ (D=0) Tally ouput after every batch. D=0 not output, D=1 output in same file

$ Cut-off energy
emin(1) = 1.0e-3 $ (D=1.0) cut-off energy for proton (MeV)
emin(2) = 1.e-10 $ (D=1.0) cut-off energy for neutron (MeV)
emin(12) = 1.e-1 # (D=1.d9) cut-off energy of electron (MeV)
emin(13) = 1.e-1 # (D=1.d9) cut-off energy of positron (MeV)
emin(14) = 1.e-3 # (D=1.d9) cut-off energy of photon (MeV)
emin(15) = 2.0e-3 # (D=1.d9) cut-off energy of deuteron (MeV/nucleon)
emin(16) = 3.0e-3 # (D=1.d9) cut-off energy of triton (MeV/nucleon)
emin(17) = 3.0e-3 # (D=1.d9) cut-off energy of 3He (MeV/nucleon)
emin(18) = 4.0e-3 # (D=1.d9) cut-off energy of Alpha (MeV/nucleon)
emin(19) = 1.0e-3 # (D=1.d9) cut-off energy of Heavy Ion (MeV/nucleon)

$ Maximum energy of nulcear data library used
$ By default, PHITS omits electron/positron/photon transport & uses Boltzmann transport for low-energy neutrons (<20MeV)
dmax(2) = 20.0 $ Neutron
dmax(12) = 1.0 $ Electron
dmax(13) = 1.0 $ positron
dmax(14) = 1.0 $ photon

$ Option for nuclear reactions
e-mode = 1 $ (D=0) Option for event-generator: 0=OFF, 1=ON
igamma = 1 $ (D=0) Option for gamma decay for residual nuclei: 0=no decay, 1=use 'trxcrd.dat', 2=EBITIM model, 3=EBITIM+isomer production
ipnint = 1 $ (D=0) Option for photonuclear reaction: 0=OFF, 1=ON
file(7) = data/xsdir.jnd $ Cross section data library for low energy neutrons
file(14)= data/trxcrd.dat $ Cross section data library for photon emission from residual nuclei

$ Option for charged particle transport
nedisp = 1 $ (D=0) Energy straggling: 0=OFF, 1=Landau-Vavilov
nspred = 2 $ (D=0) Angle straggling: 0=OFF, 2=Moliere First Coulomb diffusion
itstep = 1 $ (D=0) Option for timing tally "correct" curvature for momentum changing trajectory e.g. in magnetic field

$
%%

```
[source]
s-type  = 1              % Source type: 1=cylinder, 2=rectangular, 9=spherical
proj    = 2112           % Projectile: 2112=neutron
dir     = 1              % Initial direction relative to positive-z axis: dir=cosine
e0      = 2.45           % Initial energy (MeV)

x0     = 0
y0     = 0
z0      = 0.             % zmin (cm)
z1      = 0.             % zmax:  z1=z0 circle plan source
r0      = 1.7            % radius of the cylindrical source

$
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%
[material]
$ Material composition info: nuclei & density
$ Density can be defined in [cell], then in [material] you only need to define material
compositions
$ i.e. weight fractions, if density is defined in g/cm^3, or atomic fractions if density in
10^24 atoms/cm^3
$ Library number and data class in "data/xsdir.jnd"

 MAT[1] $ Lead, den = 11.35 g/cc
        82204.50c       -0.01378
        82206.50c       -0.23955
        82207.50c       -0.22074
        82208.50c       -0.52592

 MAT[2] $ Titanium trifluoride, den = 3.4 g/cc
       22048.50c          -0.336517056
         22046.50c        -0.037655035
         22049.50c        -0.024691003
         22047.50c        -0.033948418
         22050.50c        -0.023668488
         9019.50c         -0.54352

 MAT[3] $ Aluminium Fluoride, den = 2.88 g/cc
       13027.50c        -0.32130
       9019.50c         -0.67870

 MAT[4] $ Dry air, den=0.001205g/cc
          6000.50c      -0.000124
          7014.50c      -0.752291
          7015.50c      -0.002977
          8016.50c      -0.231781
       18040.50c        -0.012827
```

```
 $
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
 [mat name color]
 mat     name              size      color
 0         void               1          white
 1         Pb                  1          camel
 2         TiF3            1       pink
 3      AlF3           1       green
 4      air            1       blue

$
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
[ S u r f a c e ]
  10  so     500.
  11  cz       20.                   $ 20 cm radius of Pb and 4 cm thickness
  12  pz       0.
  13  pz       4.
  14  cz       20.                   $ 20 cm radius of Tif3 and 16 cm thickness
  15  pz       4.
  16  pz       20.
  17  cz       20.                   $ 20 cm radius of AlF3 and 60 cm thickness
  18  pz       20.
  19  pz       80.
  20  sph      0 0 0 1                 $ Air 1 cm radius, detector

$
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
[cell]
$ If density is positive: unit 10^24 atoms/cm^3 (= atoms/barn/cm)
$ If density is negative: unit g/cm^3

$id     mat     den              surface
 100    -1       10
  101   1        -11.35       -11  12  -13
  102   2        -3.4         -14  15  -16
  103   3        -2.88        -17  18  -19
  104   4            -0.001205    -20                    trcl=(0 0 81)
  110   0        -10   #101  #102  #103 #104                     $ working area

 $
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
 [volume]
```

```
 reg              vol
 101              5024.          $ cell 1
 102              20096.
 103          75360.
 104          4.19

$
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%
[ T - product ]off        $ Check product-eng

mesh    = reg
reg     = {101-105}

e-type  = 3                              $ (=3) log scale
ne      = 50
emin    = 1.e-8
emax    = 100.                           $ MeV

mother  = all

part    = Neutron Photon
unit    = 1                              $ 1/source

axis   =  eng
file   =  product-eng.dat
gshow  =  3
epsout =  1
resol  =  1

[t-track] off             $xy: check geometry
$Region crossing tally

mesh   = xyz

z-type = 1
nz     = 3
          -5 0 10 20 30 45

x-type = 2
nx     = 100
xmin   = -15
xmax   = 15

y-type = 2
ny     = 100
ymin   = -15
```

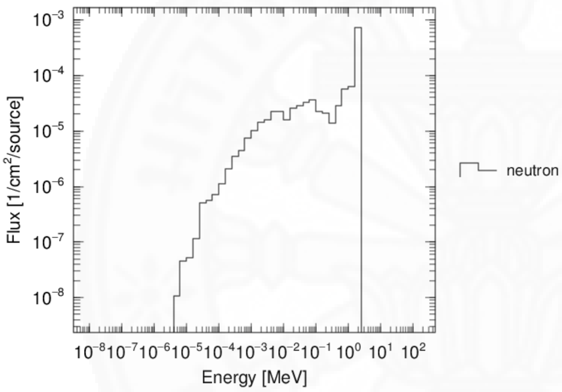
```
ymax   = 15

e-type = 3                          $ All energies
ne     = 1
emin   = 1e-8
emax   = 1e2                        $ MeV

part   = Neutron Photon                    $ 2112=neutron 22=photon
unit   = 1                          $ 1/cm^2/source

axis   = xy
file   = track-xy.dat               $ all particles in one diagram
gshow  = 3                          $ 2: region boundary & material name; 3: region
boundary and name
epsout = 1
resol  = 1

$
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%
[t-track] off             $yz: check geometry
$Region crossing tally

mesh   = xyz

x-type = 1
nx     = 3
          -30 -10 +10 +30

y-type = 2
ny     = 100
ymin   = -30
ymax   = 30

z-type = 2
nz     = 100
zmin   = -5
zmax   = 60

e-type = 3                          $ All energies
ne     = 1
emin   = 1e-8
emax   = 1e2                        $ MeV

part   = Neutron Photon                    $ 2112=neutron 22=photon
unit   = 1                          $ 1/cm^2/source
```

```
axis   = yz
file   = track-yz.dat                    $ all particles in one diagram
gshow  = 3                               $ 2: region boundary & material name; 3: region
boundary and region name
epsout = 1
resol  = 1

$
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%
[T-track]                        $ Tally particle energies in detectors
$ Region crossing tally

mesh    = reg
reg     = {101-104}
e-type  = 3                              $ (=3) log scale
ne      = 50
emin    = 1.e-8
emax    = 100.                           $ MeV

part    = Neutron                $ 2112=neutron, 22=photon, 2212=proton
unit    = 1                              $ 1/cm^2/source

axis    = eng
file    = track-reg-eng-DD2mode60.dat               $ all particles in one diagram
gshow   = 3                              $ 2: region boundary & material name; 3: region
boundary and name
epsout  = 1
resol   = 1

$
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%
[ T - product ]  off      $ Check source xy

mesh   = xyz

z-type = 1
nz     = 3
         -5 0 10 20 30 45

x-type = 2
nx     = 100
xmin   = -30
xmax   = 30

y-type = 2
```

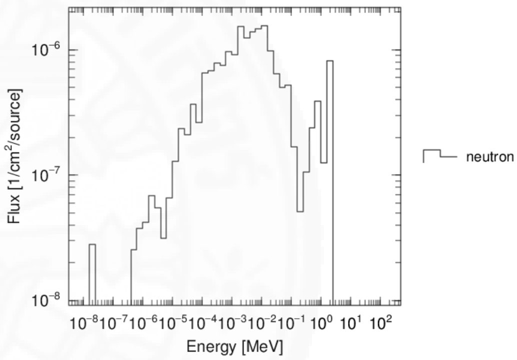
```
ny     = 100
ymin   = -30
ymax   = 30

e-type = 3                              $ All energies
ne     = 1
emin   = 1.e-8
emax   = 100.0                          $ MeV

part   =  neutron
unit   =  1                             $ (=1) 1/source, (=2) 1/cm^3/source
output =  source

axis   =  xy
file   =  source-xy.dat
gshow  =  3
epsout =  1
resol  =  1

[ T - Gshow ] off
    mesh =  xyz           # mesh type is xyz scoring mesh
  x-type =    2           # x-mesh is linear given by xmin, xmax and nx
      nx =   50           # number of x-mesh points
    xmin =  -25.          # minimum value of x-mesh points
    xmax =   25.          # maximum value of x-mesh points
  y-type =    2           # y-mesh is linear given by ymin, ymax and ny
      ny =   50           # number of y-mesh points
    ymin =  -25.          # minimum value of y-mesh points
    ymax =   25.          # maximum value of y-mesh points
  z-type =    1           # z-mesh is given by the below data
      nz =    1           # number of z-mesh points
          0.0  25.0
    axis =   xy           # axis of output
  output =    6           # (D=2) 1:bnd, 2:bnd+mat, 3:bnd+num 4:bnd+mat+num
    file = xy_gshow.dat    # file name of output for the above axis
   title = Check geometry using [T-gshow] tally
  epsout =    1           # (D=0) generate eps file by ANGEL

[ T - Gshow ] off
    mesh =  xyz           # mesh type is xyz scoring mesh
  x-type =    2           # x-mesh is linear given by xmin, xmax and nx
      nx =   50           # number of x-mesh points
    xmin =  -25.          # minimum value of x-mesh points
    xmax =   25.          # maximum value of x-mesh points
  y-type =    1           # y-mesh is given by the below data
      ny =    1           # number of y-mesh points
          -25.0  25.0
```

```
  z-type =    2            # z-mesh is linear given by zmin, zmax and nz
      nz =   50            # number of z-mesh points
    zmin =  -10.           # minimum value of z-mesh points
    zmax =   80.           # maximum value of z-mesh points
    axis =   xz            # axis of output
  output =    6            # (D=2) 1:bnd, 2:bnd+mat, 3:bnd+num 4:bnd+mat+num
    file = xz_gshow.dat    # file name of output for the above axis
   title = Check geometry using [T-gshow] tally
  epsout =    1            # (D=0) generate eps file by ANGEL
$
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
[end]
```

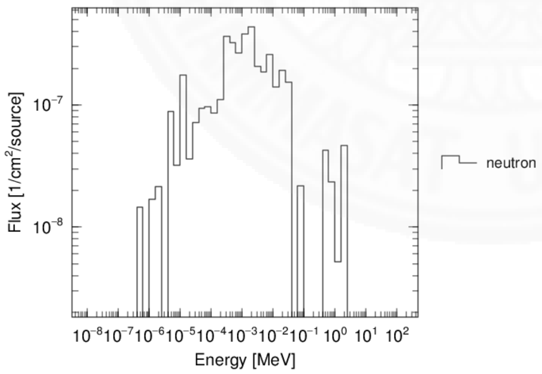
3.2. T-Track



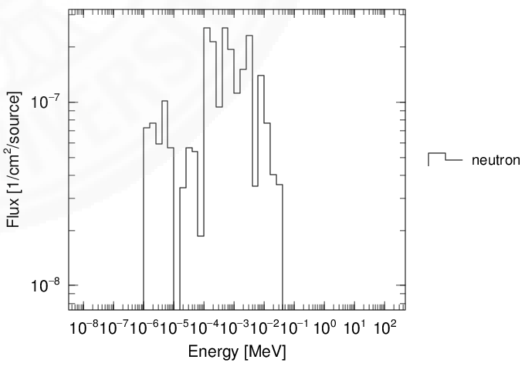
4 cm



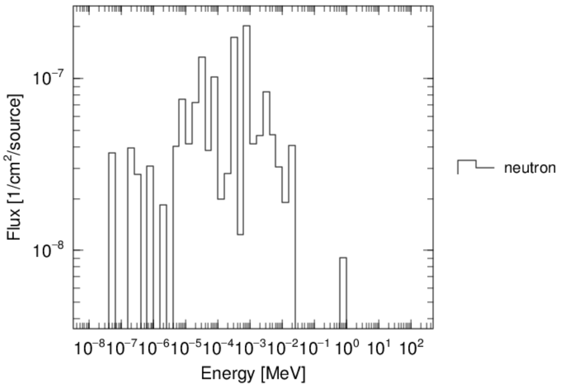
36 cm



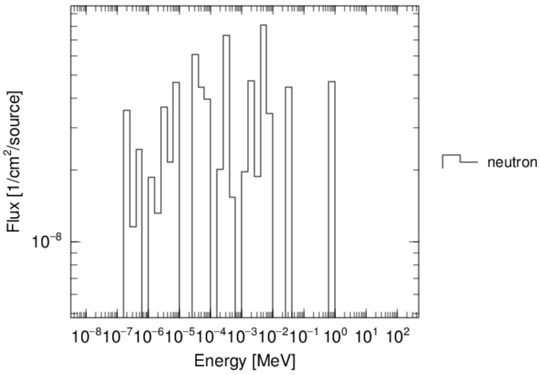
50 cm



55 cm



60 cm



65 cm

4. Al_2O_3 as a reflector
4.1 input file

```
[title]
Example 1: Get started
$ "D" = default value
$ Comments with '$', '#', 'c'

$
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
[parameters]          $ Simulation parameters
file(6)  = phits.out  $ Output filename
maxcas   = 1e7        $ Number of events per batch
maxbch   = 1          $ Number of batch
imout    = 2          $ Option of material representation in [material] 2:MCNP-type
icntl    = 0          $ (D=0)Calculation mode: 0=real simulation, 5=no reactions (void all), 6=source check, 8=check geometry
itall    = 1          $ (D=0) Tally ouput after every batch. D=0 not output, D=1 output in same file

$ Cut-off energy
emin(1)  = 1.0e-3     $ (D=1.0) cut-off energy for proton (MeV)
emin(2)  = 1.e-10     $ (D=1.0) cut-off energy for neutron (MeV)
emin(12) = 1.e-1      # (D=1.d9) cut-off energy of electron (MeV)
emin(13) = 1.e-1      # (D=1.d9) cut-off energy of positron (MeV)
emin(14) = 1.e-3      # (D=1.d9) cut-off energy of photon (MeV)
emin(15) = 2.0e-3     # (D=1.d9) cut-off energy of deuteron (MeV/nucleon)
emin(16) = 3.0e-3     # (D=1.d9) cut-off energy of triton (MeV/nucleon)
emin(17) = 3.0e-3     # (D=1.d9) cut-off energy of 3He (MeV/nucleon)
emin(18) = 4.0e-3     # (D=1.d9) cut-off energy of Alpha (MeV/nucleon)
emin(19) = 1.0e-3     # (D=1.d9) cut-off energy of Heavy Ion (MeV/nucleon)

$ Maximum energy of nulcear data library used
```

```
$ By default, PHITS omits electron/positron/photon transport & uses Boltzmann
transport for low-energy neutrons (<20MeV)
dmax(2)  = 20.0                 $ Neutron
dmax(12) = 1.0                  $ Electron
dmax(13) = 1.0                  $ positron
dmax(14) = 1.0                  $ photon

$ Option for nuclear reactions
e-mode  = 1              $ (D=0) Option for event-generator: 0=OFF, 1=ON
igamma  = 1              $ (D=0) Option for gamma decay for residual nuclei: 0=no
decay, 1=use 'trxcrd.dat', 2=EBITIM model, 3=EBITIM+isomer production
ipnint  = 1       $ (D=0) Option for photonuclear reaction: 0=OFF, 1=ON
file(7) = data/xsdir.jnd         $ Cross section data library for low energy neutrons
file(14)= data/trxcrd.dat        $ Cross section data library for photon emission from
residual nuclei

$ Option for charged particle transport
nedisp   = 1             $ (D=0) Energy straggling: 0=OFF, 1=Landau-Vavilov
nspred   = 2             $ (D=0) Angle straggling: 0=OFF, 2=Moliere First Coulomb
diffusion
itstep   = 1             $ (D=0) Option for timing tally "correct" curvature for
momentum changing trajectory e.g. in magnetic field

$
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%
[source]
s-type  = 1              % Source type: 1=cylinder, 2=rectangular, 9=spherical
proj     = 2112          % Projectile: 2112=neutron
dir      = 1             % Initial direction relative to positive-z axis: dir=cosine
e0       = 2.45          % Initial energy (MeV)

x0     = 0
y0     = 0
z0       = 0.            % zmin (cm)
z1       = 0.            % zmax:  z1=z0 circle plan source
r0       = 1.7           % radius of the cylindrical source

$
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%
[material]
$ Material composition info: nuclei & density
$ Density can be defined in [cell], then in [material] you only need to define material
compositions
$ i.e. weight fractions, if density is defined in g/cm^3, or atomic fractions if density in
10^24 atoms/cm^3
```

```
$ Library number and data class in "data/xsdir.jnd"

 MAT[1] $ Lead, den = 11.35 g/cc
        82204.50c       -0.01378
        82206.50c       -0.23955
        82207.50c       -0.22074
        82208.50c       -0.52592

MAT[2] $ Titanium trifluoride, den = 3.4 g/cc
      22048.50c          -0.336517056
         22046.50c       -0.037655035
         22049.50c       -0.024691003
         22047.50c       -0.033948418
         22050.50c       -0.023668488
         9019.50c        -0.54352

MAT[3] $ Aluminium Fluoride, den = 2.88 g/cc
       13027.50c        -0.32130
       9019.50c         -0.67870

MAT[4] $ Aluminum Oxide, den = 3.97 g/cc
       8016.50c        -0.470749
      13027.50c        -0.52925

MAT[5] $ Dry air, den=0.001205g/cc
          6000.50c      -0.000124
          7014.50c      -0.752291
          7015.50c      -0.002977
          8016.50c      -0.231781
         18040.50c      -0.012827

$
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%
[mat name color]
mat    name          size    color
0      void          1       white
1      Pb            1       camel
2      TiF3          1     pink
3     AlF3           1     green
4     Al2O3          1     yellow
5     air            1     blue

$
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%
[ S u r f a c e ]
```

```
 10  so     500.
 11  cz       20.                 $ 20 cm radius of Pb and 4 cm thickness
 12  pz       0.
 13  pz       4.
 14  cz       20.                 $ 20 cm radius of Tif3 and 16 cm thickness
 15  pz       4.
 16  pz       20.
 17  cz       20.                 $ 20 cm radius of AlF3 and 60 cm thickness
 18  pz       20.
 19  pz       80.
 20  cz       30.                 $ 30 cm radius of Al2O3 and 80 cm as a reflector
 21  pz        0.
 22  pz       80.
 23  sph      0 0 0 1             $ Air 1 cm radius, detector

$
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
[cell]
$ If density is positive: unit 10^24 atoms/cm^3 (= atoms/barn/cm)
$ If density is negative: unit g/cm^3

$id    mat    den           surface
 100   -1      10
  101   1      -11.35        -11  12  -13
  102   2      -3.4          -14  15  -16
  103   3      -2.88         -17  18  -19
  104   4      -3.97         -20  21  -22            #101  #102  #103
  105   5      -0.001205     -23                  trcl=(0 0 81)
  110   0      -10   #101  #102  #103 #104  #105                    $ working area

 $
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
 [volume]
 reg              vol
 101              5024.          $ cell 1
 102              20096.
 103             75360.
 104            125600.
 105            4.19

$
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
[ T - product ]off       $ Check product-eng
```

```
mesh    = reg
reg     = {101-105}

e-type  = 3                          $ (=3) log scale
ne      = 50
emin    = 1.e-8
emax    = 100.                       $ MeV

mother  = all

part    = Neutron Photon
unit    = 1                          $ 1/source

axis   =  eng
file   =  product-eng.dat
gshow  =  3
epsout =  1
resol  =  1

[t-track] off          $xy: check geometry
$Region crossing tally

mesh   = xyz

z-type = 1
nz     = 3
         -5 0 10 20 30 45

x-type = 2
nx     = 100
xmin   = -15
xmax   = 15

y-type = 2
ny     = 100
ymin   = -15
ymax   = 15

e-type = 3                           $ All energies
ne     = 1
emin   = 1e-8
emax   = 1e2                         $ MeV

part   = Neutron Photon                     $ 2112=neutron 22=photon
unit   = 1                           $ 1/cm^2/source

axis   = xy
```

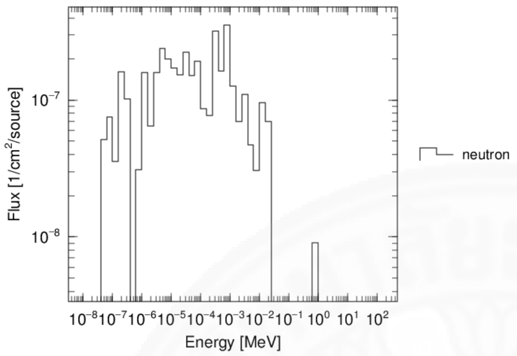
```
file   = track-xy.dat                    $ all particles in one diagram
gshow  = 3                               $ 2: region boundary & material name; 3: region
boundary and name
epsout = 1
resol  = 1

$
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%
[t-track] off              $yz: check geometry
$Region crossing tally

mesh   = xyz

x-type = 1
nx     = 3
         -30 -10 +10 +30

y-type = 2
ny     = 100
ymin   = -30
ymax   = 30

z-type = 2
nz     = 100
zmin   = -5
zmax   = 60

e-type = 3                               $ All energies
ne     = 1
emin   = 1e-8
emax   = 1e2                             $ MeV

part   = Neutron Photon                          $ 2112=neutron 22=photon
unit   = 1                               $ 1/cm^2/source

axis   = yz
file   = track-yz.dat                    $ all particles in one diagram
gshow  = 3                               $ 2: region boundary & material name; 3: region
boundary and region name
epsout = 1
resol  = 1

$
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%
[T-track]                        $ Tally particle energies in detectors
```

```
$ Region crossing tally

mesh    = reg
reg     = {101-105}
e-type  = 3                              $ (=3) log scale
ne      = 50
emin    = 1.e-8
emax    = 100.                           $ MeV

part    = Neutron                  $ 2112=neutron, 22=photon, 2212=proton
unit    = 1                              $ 1/cm^2/source

axis    = eng
file    = track-reg-eng-DD2ref30o.dat          $ all particles in one diagram
gshow   = 3                              $ 2: region boundary & material name; 3: region
boundary and name
epsout  = 1
resol   = 1

$
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%
[ T - product ]  off      $ Check source xy

mesh   = xyz

z-type = 1
nz     = 3
          -5 0 10 20 30 45

x-type = 2
nx     = 100
xmin   = -30
xmax   = 30

y-type = 2
ny     = 100
ymin   = -30
ymax   = 30

e-type = 3                               $ All energies
ne     = 1
emin   = 1.e-8
emax   = 100.0                           $ MeV

part   =  neutron
unit   =  1                              $ (=1) 1/source, (=2) 1/cm^3/source
```

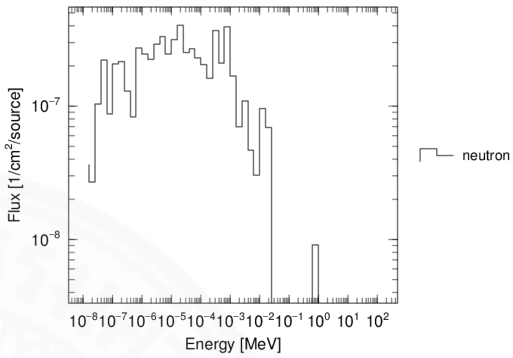
```
output =  source

axis   =  xy
file   =  source-xy.dat
gshow  =  3
epsout =  1
resol  =  1

[ T - Gshow ] off
    mesh =  xyz          # mesh type is xyz scoring mesh
  x-type =    2          # x-mesh is linear given by xmin, xmax and nx
      nx =   50          # number of x-mesh points
    xmin =  -25.          # minimum value of x-mesh points
    xmax =   25.          # maximum value of x-mesh points
  y-type =    2          # y-mesh is linear given by ymin, ymax and ny
      ny =   50          # number of y-mesh points
    ymin =  -25.          # minimum value of y-mesh points
    ymax =   25.          # maximum value of y-mesh points
  z-type =    1          # z-mesh is given by the below data
      nz =    1          # number of z-mesh points
         0.0  25.0
    axis =   xy          # axis of output
  output =    6          # (D=2) 1:bnd, 2:bnd+mat, 3:bnd+num 4:bnd+mat+num
    file = xy_gshow.dat    # file name of output for the above axis
   title = Check geometry using [T-gshow] tally
  epsout =    1          # (D=0) generate eps file by ANGEL

[ T - Gshow ] off
    mesh =  xyz          # mesh type is xyz scoring mesh
  x-type =    2          # x-mesh is linear given by xmin, xmax and nx
      nx =   50          # number of x-mesh points
    xmin =  -25.          # minimum value of x-mesh points
    xmax =   25.          # maximum value of x-mesh points
  y-type =    1          # y-mesh is given by the below data
      ny =    1          # number of y-mesh points
         -25.0  25.0
  z-type =    2          # z-mesh is linear given by zmin, zmax and nz
      nz =   50          # number of z-mesh points
    zmin =  -10.          # minimum value of z-mesh points
    zmax =   80.          # maximum value of z-mesh points
    axis =   xz          # axis of output
  output =    6          # (D=2) 1:bnd, 2:bnd+mat, 3:bnd+num 4:bnd+mat+num
    file = xz_gshow.dat    # file name of output for the above axis
   title = Check geometry using [T-gshow] tally
  epsout =    1          # (D=0) generate eps file by ANGEL
```

$
%%
%%%%%%%%%%%
[end]

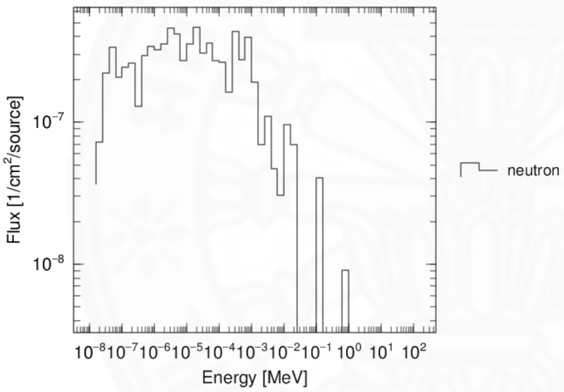
4.2 [t-track]



25 cm



30 cm



35 cm

5. Li as the thermal neutron filter
5.1 input file

[title]
Example 1: Get started
$ "D" = default value
$ Comments with '$', '#', 'c'

$
%%
%%%%%%%%%%%
[parameters] $ Simulation parameters
file(6) = phits.out $ Output filename
maxcas   = 1e8 $ Number of events per batch
maxbch   = 1 $ Number of batch
imout   = 2 $ Option of material representation in [material] 2:MCNP-type

icntl = 0 $ (D=0)Calculation mode: 0=real simulation, 5=no reactions (void all), 6=source check, 8=check geometry
itall = 1 $ (D=0) Tally ouput after every batch. D=0 not output, D=1 output in same file

$ Cut-off energy
emin(1) = 1.0e-3 $ (D=1.0) cut-off energy for proton (MeV)
emin(2) = 1.e-10 $ (D=1.0) cut-off energy for neutron (MeV)
emin(12) = 1.e-1 # (D=1.d9) cut-off energy of electron (MeV)
emin(13) = 1.e-1 # (D=1.d9) cut-off energy of positron (MeV)
emin(14) = 1.e-3 # (D=1.d9) cut-off energy of photon (MeV)
emin(15) = 2.0e-3 # (D=1.d9) cut-off energy of deuteron (MeV/nucleon)
emin(16) = 3.0e-3 # (D=1.d9) cut-off energy of triton (MeV/nucleon)
emin(17) = 3.0e-3 # (D=1.d9) cut-off energy of 3He (MeV/nucleon)
emin(18) = 4.0e-3 # (D=1.d9) cut-off energy of Alpha (MeV/nucleon)
emin(19) = 1.0e-3 # (D=1.d9) cut-off energy of Heavy Ion (MeV/nucleon)

$ Maximum energy of nulcear data library used
$ By default, PHITS omits electron/positron/photon transport & uses Boltzmann transport for low-energy neutrons (<20MeV)
dmax(2) = 20.0 $ Neutron
dmax(12) = 1.0 $ Electron
dmax(13) = 1.0 $ positron
dmax(14) = 1.0 $ photon

$ Option for nuclear reactions
e-mode = 1 $ (D=0) Option for event-generator: 0=OFF, 1=ON
igamma = 1 $ (D=0) Option for gamma decay for residual nuclei: 0=no decay, 1=use 'trxcrd.dat', 2=EBITIM model, 3=EBITIM+isomer production
ipnint = 1 $ (D=0) Option for photonuclear reaction: 0=OFF, 1=ON
file(7) = data/xsdir.jnd $ Cross section data library for low energy neutrons
file(14)= data/trxcrd.dat $ Cross section data library for photon emission from residual nuclei

$ Option for charged particle transport
nedisp = 1 $ (D=0) Energy straggling: 0=OFF, 1=Landau-Vavilov
nspred = 2 $ (D=0) Angle straggling: 0=OFF, 2=Moliere First Coulomb diffusion
itstep = 1 $ (D=0) Option for timing tally "correct" curvature for momentum changing trajectory e.g. in magnetic field

$
%%%
[source]
s-type = 1 % Source type: 1=cylinder, 2=rectangular, 9=spherical
proj = 2112 % Projectile: 2112=neutron

```
dir       = 1               % Initial direction relative to positive-z axis: dir=cosine
e0        = 2.45            % Initial energy (MeV)

x0     = 0
y0     = 0
z0        = 0.              % zmin (cm)
z1        = 0.              % zmax:  z1=z0 circle plan source
r0        = 1.7             % radius of the cylindrical source

$
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%
[material]
$ Material composition info: nuclei & density
$ Density can be defined in [cell], then in [material] you only need to define material
compositions
$ i.e. weight fractions, if density is defined in g/cm^3, or atomic fractions if density in
10^24 atoms/cm^3
$ Library number and data class in "data/xsdir.jnd"

 MAT[1] $ Lead, den = 11.35 g/cc
        82204.50c       -0.01378
        82206.50c       -0.23955
        82207.50c       -0.22074
        82208.50c       -0.52592

MAT[2] $ Titanium trifluoride, den = 3.4 g/cc
       22048.50c            -0.336517056
          22046.50c         -0.037655035
          22049.50c         -0.024691003
          22047.50c         -0.033948418
          22050.50c         -0.023668488
          9019.50c          -0.54352

MAT[3] $ Aluminium Fluoride, den = 2.88 g/cc
        13027.50c         -0.32130
        9019.50c      -0.67870

MAT[4] $ Aluminum Oxide, den = 3.97 g/cc
        8016.50c         -0.470749
       13027.50c          -0.52925

MAT[5] $ Lithium, den = 0.534 g/cc
      3006.50c        -0.075
      3007.50c              -0.925

MAT[6] $ Dry air, den=0.001205g/cc
```

```
           6000.50c       -0.000124
           7014.50c       -0.752291
           7015.50c       -0.002977
           8016.50c       -0.231781
          18040.50c       -0.012827

 $
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%
 [mat name color]
 mat    name          size    color
 0       void          1      white
 1       Pb            1      camel
 2       TiF3          1      pink
 3     AlF3           1       green
 4     Al2O3          1       yellow
 5     Li             1        brown
 6     air            1       blue

$
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%
[ S u r f a c e ]
  10  so    500.
  11  cz      20.                    $ 20 cm radius of Pb and 4 cm thickness
  12  pz      0.
  13  pz      4.
  14  cz      20.                    $ 20 cm radius of Tif3 and 16 cm thickness
  15  pz      4.
  16  pz      20.
  17  cz      20.                    $ 20 cm radius of AlF3 and 60 cm thickness
  18  pz      20.
  19  pz      80.
  20  cz      30.                    $ 30 cm radius of Al2O3 and 83 cm as a reflector
  21  pz       0.
  22  pz      83.
  23  TRC     0. 0. 0. 0. 0. 3.  20.  14.      $ Li and 3 cm thickness, r1=20 cm, r2=14
cm
  24  sph     0 0 0 1                  $ Air 1 cm radius, detector

$
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%
[cell]
$ If density is positive: unit 10^24 atoms/cm^3 (= atoms/barn/cm)
$ If density is negative: unit g/cm^3
```

```
$id    mat    den             surface
 100   -1      10
  101   1      -11.35         -11  12  -13
  102   2      -3.4           -14  15  -16
  103   3      -2.88          -17  18  -19
  104   4      -3.97          -20  21  -22          #101  #102  #103 #105
  105   5      -0.534         -23               trcl=(0 0 80)
  106   6      -0.001205      -24               trcl=(0 0 84)
  110   0      -10   #101  #102  #103 #104  #105 #106                  $ working area

 $
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%
 [volume]
 reg            vol
 101            5024.          $ cell 1
 102            20096.
 103           75360.
 104           131325.97
 105            2752.03
 106            4.19

$
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%
[ T - product ]off       $ Check product-eng

mesh    = reg
reg     = {101-105}

e-type  = 3                         $ (=3) log scale
ne      = 50
emin    = 1.e-8
emax    = 100.                      $ MeV

mother  = all

part    = Neutron Photon
unit    = 1                         $ 1/source

axis   =  eng
file   =  product-eng.dat
gshow  =  3
epsout =  1
resol  =  1

[t-track] off            $xy: check geometry
```

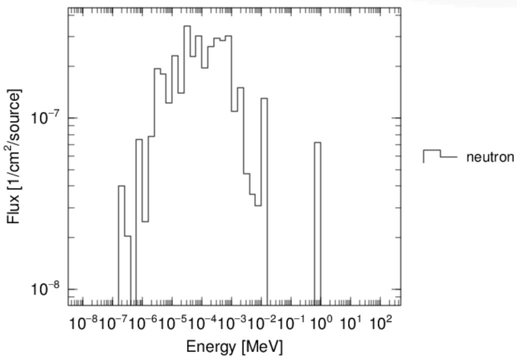
```
$Region crossing tally

mesh   = xyz

z-type = 1
nz     = 3
         -5 0 10 20 30 45

x-type = 2
nx     = 100
xmin   = -15
xmax   = 15

y-type = 2
ny     = 100
ymin   = -15
ymax   = 15

e-type = 3                              $ All energies
ne     = 1
emin   = 1e-8
emax   = 1e2                            $ MeV

part   = Neutron Photon                          $ 2112=neutron 22=photon
unit   = 1                              $ 1/cm^2/source

axis   = xy
file   = track-xy.dat                   $ all particles in one diagram
gshow  = 3                              $ 2: region boundary & material name; 3: region
boundary and name
epsout = 1
resol  = 1

$
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%
[t-track] off          $yz: check geometry
$Region crossing tally

mesh   = xyz

x-type = 1
nx     = 3
         -30 -10 +10 +30

y-type = 2
ny     = 100
```

```
ymin   = -30
ymax   = 30

z-type = 2
nz     = 100
zmin   = -5
zmax   = 60

e-type = 3                              $ All energies
ne     = 1
emin   = 1e-8
emax   = 1e2                            $ MeV

part   = Neutron Photon                         $ 2112=neutron 22=photon
unit   = 1                              $ 1/cm^2/source

axis   = yz
file   = track-yz.dat                   $ all particles in one diagram
gshow  = 3                              $ 2: region boundary & material name; 3: region
boundary and region name
epsout = 1
resol  = 1

$
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%
[T-track]                       $ Tally particle energies in detectors
$ Region crossing tally

mesh    = reg
reg     = {101-106}
e-type  = 3                             $ (=3) log scale
ne      = 50
emin    = 1.e-8
emax    = 100.                          $ MeV

part    = Neutron                       $ 2112=neutron, 22=photon, 2212=proton
unit    = 1                             $ 1/cm^2/source

axis    = eng
file    = track-reg-eng-DD2th3.dat              $ all particles in one diagram
gshow   = 3                             $ 2: region boundary & material name; 3: region
boundary and name
epsout  = 1
resol   = 1
```

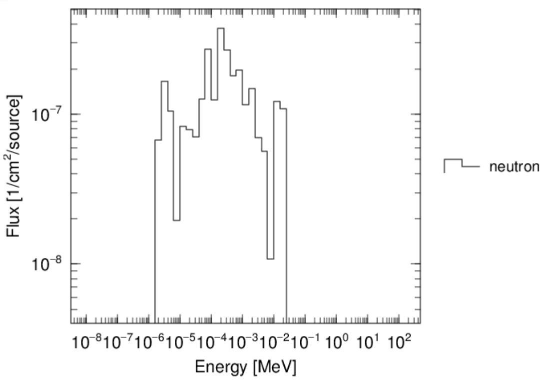
```
$
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%
[ T - product ]  off      $ Check source xy

mesh   = xyz

z-type = 1
nz     = 3
           -5 0 10 20 30 45

x-type = 2
nx     = 100
xmin   = -30
xmax   = 30

y-type = 2
ny     = 100
ymin   = -30
ymax   = 30

e-type = 3                                   $ All energies
ne     = 1
emin   = 1.e-8
emax   = 100.0                               $ MeV

part   =  neutron
unit   =  1                                  $ (=1) 1/source, (=2) 1/cm^3/source
output =  source

axis   =  xy
file   =  source-xy.dat
gshow  =  3
epsout =  1
resol  =  1

[ T - Gshow ] off
    mesh =  xyz          # mesh type is xyz scoring mesh
  x-type =    2          # x-mesh is linear given by xmin, xmax and nx
      nx =   50          # number of x-mesh points
    xmin =  -25.         # minimum value of x-mesh points
    xmax =   25.         # maximum value of x-mesh points
  y-type =    2          # y-mesh is linear given by ymin, ymax and ny
      ny =   50          # number of y-mesh points
    ymin =  -25.         # minimum value of y-mesh points
    ymax =   25.         # maximum value of y-mesh points
  z-type =    1          # z-mesh is given by the below data
```

```
      nz =    1            # number of z-mesh points
          0.0  25.0
    axis =   xy            # axis of output
  output =    6            # (D=2) 1:bnd, 2:bnd+mat, 3:bnd+num 4:bnd+mat+num
    file = xy_gshow.dat    # file name of output for the above axis
   title = Check geometry using [T-gshow] tally
  epsout =    1            # (D=0) generate eps file by ANGEL

[ T - Gshow ] off
    mesh =  xyz            # mesh type is xyz scoring mesh
  x-type =    2            # x-mesh is linear given by xmin, xmax and nx
      nx =   50            # number of x-mesh points
    xmin =  -40.           # minimum value of x-mesh points
    xmax =   40.           # maximum value of x-mesh points
  y-type =    1            # y-mesh is given by the below data
      ny =    1            # number of y-mesh points
          -25.0  25.0
  z-type =    2            # z-mesh is linear given by zmin, zmax and nz
      nz =   50            # number of z-mesh points
    zmin =  -10.           # minimum value of z-mesh points
    zmax =   100.          # maximum value of z-mesh points
    axis =   xz            # axis of output
  output =    6            # (D=2) 1:bnd, 2:bnd+mat, 3:bnd+num 4:bnd+mat+num
    file = xz_gshow.dat    # file name of output for the above axis
   title = Check geometry using [T-gshow] tally
  epsout =    1            # (D=0) generate eps file by ANGEL
$
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%
[end]
```

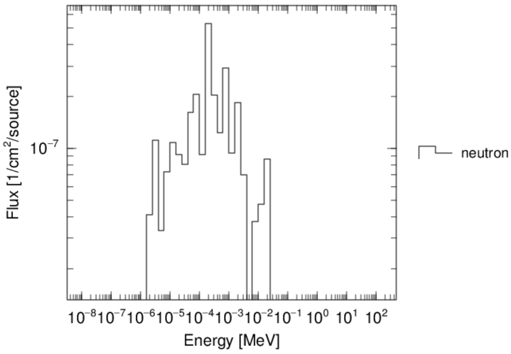
5.2. [t-track]



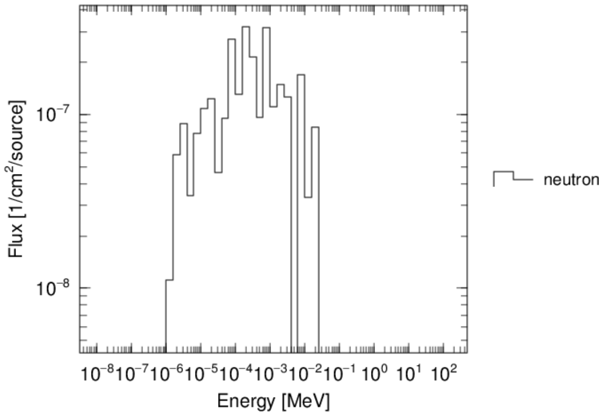
1 cm



2 cm


Flux [1/cm^2/source]
10^-7
Energy [MeV]
10^-8 10^-7 10^-6 10^-5 10^-4 10^-3 10^-2 10^-1 10^0 10^1 10^2
neutron

3 cm


Flux [1/cm^2/source]
10^-7
10^-8
Energy [MeV]
10^-8 10^-7 10^-6 10^-5 10^-4 10^-3 10^-2 10^-1 10^0 10^1 10^2
neutron

4 cm