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A simulation on desired neutron flux for the boron neutron capture therapy (BNCT) purpose by using Monte Carlo N-Particle (MCNPX)

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Abstract. Boron Neutron Capture Therapy (BNCT) is a nuclear application to cure cancer by using the interaction between the boron compound and the slow (thermal and epithermal) neutron beam obtained from the neutron source. The previous feasibility study shows that the thermal column can generate higher thermal neutrons for BNCT application at the TRIGA MARK II reactor. Currently, the BNCT facility is planned to be developed at the thermal column. Thus, to fabricate the nuclear application such as BNCT required several required such as the study of design, material, neutron desired and safety for the application. Therefore, the use of simulation software such as Monte Carlo N-Particle (MCNP) was extensively essential to identify and determine the most convenient design of the BNCT facility with proper safety requirement standard. Besides that, the simulation also useful in terms of identifying good material and best geometry and the uses of simulation can guide to make sure this research achieves the best results. Generally, MCNP function to track the particle over its energy range using the irradiation transport and the neutron flux and the gamma flux produced from the simulation using MCNPX code was consider right if the relative errors contributed was lower than 5%. This research simulates that the uncovered collimator provides high neutron flux and high collimator performance compared to the fully covered collimator. This research is useful in the simulate on the desired neutron from the BNCT facility design at the TRIGA MARK II reactor.

1. Introduction

Boron Neutron Capture Therapy or BNCT is one of the nuclear applications that involves the uses of the neutron in the application. To fabricate the nuclear application facilities, there are several requirements need to ensure the application was safe from any radiation leakage and for avoid any radiation emergency during handling, deliver and transport the nuclear application [1]. Before the fabrication, the design and material that would be used must be to study their characteristic towards the neutron and gamma-ray. Therefore, the use of simulation software such as Monte Carlo N-Particle (MCNP) [2] was significant to avoid any radiation accident in the future. In this research, the use of software and simulation plays an important part. It was used to identify and calculate the neutron and photon fluxes, and also significant as a guideline to select the best material and the design of this research. The use of simulation was extensively essential to identify and determine the most convenient

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design of the BNCT facility with proper safety requirement standard [2]. Besides that, the simulation also useful in terms of identifying good material and best geometry and the uses of simulation can guide to make sure this research achieves the best results [1]. Generally, MCNP is very useful, uniquely to determine the photon, electron and neutron to calculate the eigenvalues for the critical systems. The use of MCNP code can treat an arbitrary 3- configuration of materials in geometric cells bounded by first and second-degree surface and fourth elliptical surfaces [3]. MCNP also can be used in several transport modes which are the combination of the neutron or photon and the electron only, photon only and neutron only. In MCNPX also are set up with the range of neutron energy that can be simulated, the energy regime is from 10-11 MeV to 20 MeV for all isotopes, and the photon energy regime is from 1 keV to 1 GeV [3].

The use of MCNP in particle transport technique is a numerical experiment. This technique includes each of the following particles throughout the source as a display in figure 1. The probability distribution is randomly sampled using transport data to determine the outcome of each step of its life [4]. One of the advantages of the MCNP is that it can use generalized input of the neutron source. The neutron source provided allow users to specify the neutron source used in the simulation. According to X-5 Monte Carlo Team [5], these independent probability distributions may be specified sources variables, especially in time, position and direction and the energy. Figure 1 shows the general flowchart process of MCNP [5]. MNCP have several types and version, such as MCNP5 and MCNPX that are widely use in the nuclear industry. Based on Radiation Information Computational Centre (RCICC), there are several differences between those two MCNP that described in table 1.

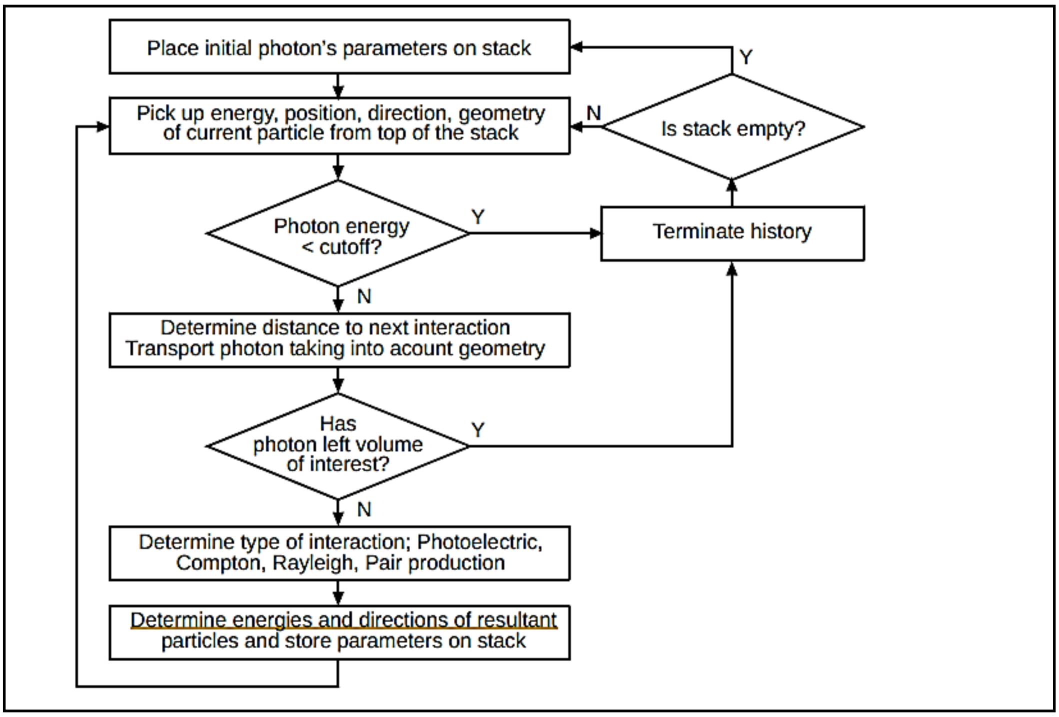

Figure 1. The general flowchart process of MCNP [5].

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Table 1. Differences between MCNP5 and MCNPX [4]

MCNP Code	Overview	Limitation
MCNP5	MCNP5 is a general-purpose code that can be used to deal with neutron transport, electron transport, gamma-ray transport, and coupled transport including eigenvalues calculation for critical systems. In MCNP5 code, thermal neutrons are interpreted by both free gas and alpha beta models while for gamma rays, the code contributes for coherent and incoherent scattering, likelihood of fluorescence emission, and absorption in electron-positron pair production. Next, both electron and positron code contribute for the Coulomb scattering angular deflection, collisional energy loss, and production of secondary particles including bremsstrahlung, annihilation of gamma rays, and electron knock-on. There are some vital features that make MCNP5 easy and versatile which are dominant general sources, surface sources and criticality sources, more variance reduction techniques, extensive cross-section data, and flexible tally structure.	The energy range for each particle are limited. For neutrons, the energy is limited from 10^{-11} to 20 MeV. For electrons, the energy are ranges from 1 keV to 1 GeV and for gamma rays, the limits are from 1 keV to 100 GeV.
MCNPX	MCNPX or MCNP eXtended is a Fortran90 radiation-transport code that can transport particles with various energy ranges. The developing of MCNPX was started in 1994 by combination of MCNP4B and LAHET2.8. It was officially released on 1999 as version 2.1.5. Then, it was upgraded to MCNP4C and converted to Fortran90 (version 2.4.0) in 2002 with added of 12 new features. Next, in 18 April 2011, MCNPX version 2.7.0 was released. Basically, MCNPX 2.7.0 is a superset of MCNP4C3 but with expanded capabilities such as tally tanging, embedded sources, cyclic time bin, and focused beam sources. Besides, there are a lot of new variance-reduction option and tally source have been created specific to the intermediate and high energy ranges. The MCNPX also was released with neutrons, gamma rays, electrons, photonuclear interaction and protons libraries.	The limitations of MCNPX are the energy ranges limited where neutrons from 0-20 MeV, gamma rays from 1 keV to 100 GeV, photonuclear interaction from 1.0 MeV to 150 MeV, electrons from 1 keV to 1 GeV, protons from 1.0 MeV to 150 MeV, light ions from 1 MeV, and heavy ions from 3 MeV.

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2. Methodology

This research is conducted using MCNPX, which only available in Nuclear Malaysia in this country for students uses. The MCNPX is user-friendly where the written code is using the coding language FOTRAN90 and can be accessed through UNIX and Windows. Besides that, MCNPX also a more accurate model of particle transport because the MCNPX package included the Vised that use to develop a geometry model even though MCNPX is the very computationally extensive and poor interface [6]. The purpose of the MCNPX uses in this research is to simulate and design the BNCT collimator based on material characterisation and selection before the fabrication. The optimum simulation of collimator design using MCNPX has been fabricated for BNCT research purpose. Before the simulation using the MCNPX software is executed, the input file must be created using the design of the collimator. Figure 2 shows a sample of the input required for collimator to be designed. This input contains the cell card, code for the type of material, density of the actual material, surface card for the collimator size and data card for a neutron source. After that, this input code has been entered into MCNPX prompt commands to be executed [6].

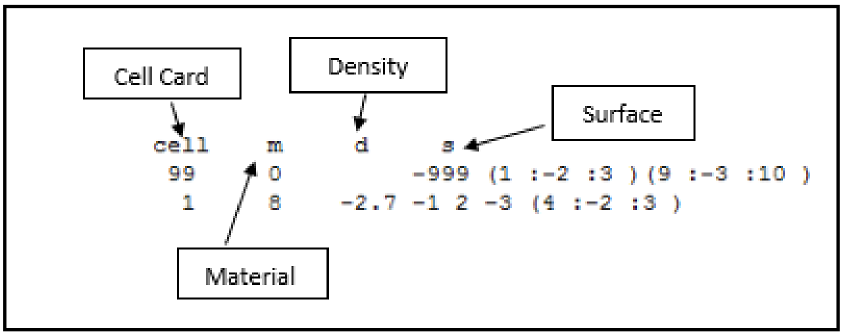

Figure 2. The cell card for MCNPX input file.

The cell card that contains code (cell number), m (material code defined in data card), d (density material), and s (surface). All those functions are used to simulate the geometry with the actual material density for the collimator. The cell card was important to identify the location of the output and the neutron source.

After the cell cards the input file of MCNPX is then followed by surface card. Figure 3 shows a surface card where this card contains the type of "macro" body involved in shaping the geometry for example the rectangular parallel-piped (RPP) geometry is for cuboid, the right circular cylinder (RCC) is in cylindrical form and the truncated right-angle cone (TRC) is cone-shaped, sphere (so), plane on x-axis (px) etc [7]. In addition to geometry, the values displayed include the range of dimensions for each geometry for each x, y and z axes [7]. The uses of Vised was important in this part to design the geometry of the collimator. To complete the input file, the data card and source card was fulfilled as shown in figure 4 and figure 5.

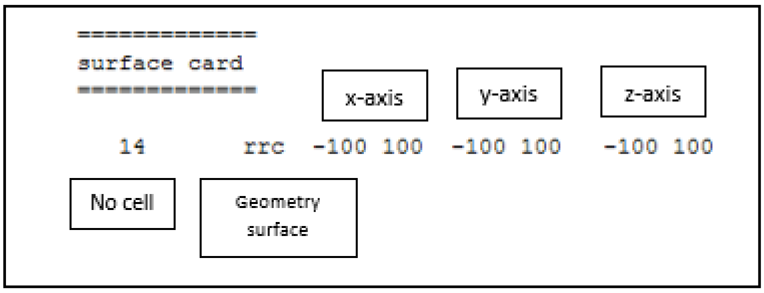

Figure 3. The surface card for MCNPX input file.

```
===========
c data card
===========
mode  p
c material
c air
m1     7014.          -0.755268  $MAT1
       8016.          -0.231781 6012.         -0.000124
c barite colemanite
m2     1001.          -0.008564  $MAT2
       5010.70c       -0.009874 8016.         -0.351537 11023.        -0.001108
       12000.         -0.002217 13027.        -0.006146 14000.        -0.017733
       16000.         -0.097028 20000.        -0.085239 25055.        -0.000101
       26000.         -0.010378 56137.        -0.410076
```

Figure 4. The data card for MCNPX input file.

The data card was important to clarify the material use for the collimator design. Any material can be added on the data card either element or compound but the element fraction must be determined to ensure the material was correct. For example, the m1 show the material air that combine two element which is nitrogen (7014) and oxygen (8016). These elements are written in the form of a numeral identification number formula or known as ZAID. This formula is written as ZZZAAA in input. ZZZ is the atomic number of an element while AAA is the mass number of elements [5].

```
============
source card
============
sdef pos=-80 0 0 sur=2 erg=d1 par=2 axs=1 0 0 dir=1 vec=1 0 0 rad=d2
si1 1 0.033 0.067
sp1 0.5 0.5
si2 0 9.5
sp2 -21 1
f4:p 13 15 16 17 20 21 2 3 4 5 6 7 9 10 11
nps 1000000000
```

Figure 5. The source card for MCNPX input file.

Figure 5 was crucial to be put into the input file. Without the source card, the MCNPX cannot simulate as there are no source and particles to be track along the collimator. In this research, the design of collimator was used Sdef as neutron source. "Sdef" is the code for a common source (general source). "Post" is a code that contains x, y and z axes to indicate where the source's initial position has been transmitted. "Axs" also refers to the axis that is parallel to the source. The value used for this code is 0 and 1. 1 0 0 means the source emitted through the x-axis, 0 1 0 means the source is transmitted through the y axis while 0 0 1 means the source is emitted in parallel to the z-axis. Next is "rad". "Rad" means the radius of a geometry that contains sources for gamma or neutrons. Normally "rad" has been defined through "si" or known as source information. "Par" refers to the particle used. 1 represents neutrons while 2 represents photons. "Erg" means the energy used in this research. The source card use in the figure 4 is the gamma source card for the collimator. Besides the source, the intended output for simulation also important. The intended output can be simply called as tally. Tally is a form of code to define the desired information. In this study, the tally used is F4 and F14 that is to find the average flux of a cell. F4: n is for neutron flux while F4: p is for photons while the F14:p is to find the secondary gamma. If tally involves a cell, the volume of a cell should be taken into account by using the sd code.

In this research 1 MW of reactor power is use. Power as much this produces particles of 4.35 x 10^{11} neutron.cm^{-2}s^{-1} particles for thermal neutrons and 4.27 x 10^{10} γcm^{-2}s^{-1} particles for gamma [8,10]. Nps used for this input is 1 billion. This value is the maximum value that can be used in MCNPX.

Nps is intended to instruct the software to stop the software. This is because the running process will stop if the nps is finished processing or fatal error on the input [5]. Figure 6 shows how to input command to command prompt for process run and to continue this step, the input header should start by typing i for input code and o for output code.

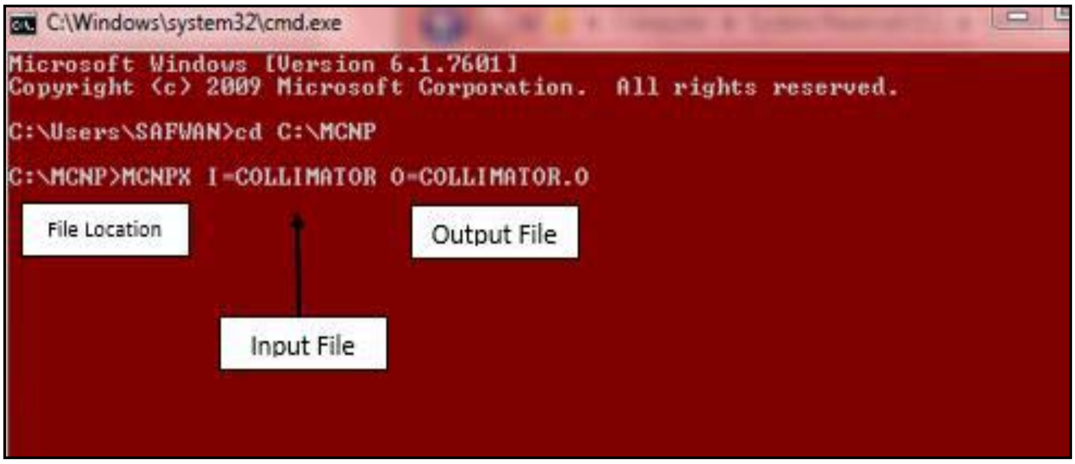

Figure 6. The input file and output file command for MCNPX.

3. Result and discussion

To select an ideal collimator for BNCT facility at the thermal column, there are several studies performed based on D1 design using MCNPX software. The studies of collimator were included the difference between the uncovered collimator and the fully covered collimator, the collimator performance and were simulate using MCNPX.

3.1. The different between uncovered and full covered collimator using MCNPX

There are two types of a collimator that can be selected, first is the uncovered collimator which has holes inside the collimator such as D1 design. The fully covered means the collimator do not have any holes besides of aperture. The main difference is, the fully covered collimator was entirely filtering the beam before collimating the beam whereas the uncovered collimator was maintaining the beam and collimate the beam. The 3 cm of aperture size with same lead thickness and same material (lead. 30% BPE, HDPE and aluminium) used for both collimators. Figure 7 shows the simulation result for both collimators on producing thermal neutron.

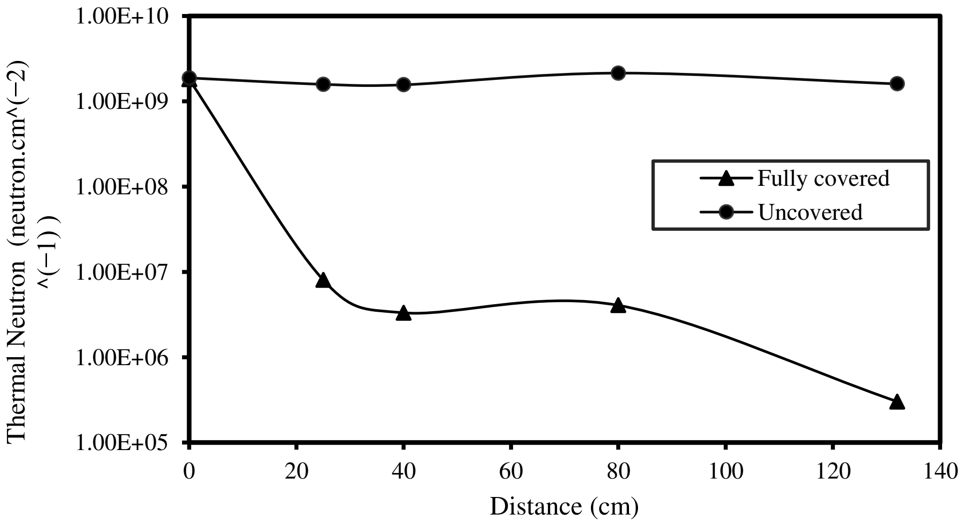

Figure 7. The different between thermal neutron produce over distance by fully covered collimator and uncovered collimator using MCNPX.

Figure 7 shows the fully covered collimator had decreased compared to uncovered collimator with about 99% of thermal neutron reduction. The fully covered of lead, 30% BPE and HDPE on collimator had shielded and reduced the beam of thermal neutron flux. The fully covered collimator cannot collimate the beam because of the beam filtration [8] by lead and 30% BPE on part 1 of collimator while uncovered collimator had sustained the flux energy from start to end of the collimator. Figure 8 illustrates the contour plot for thermal neutron from uncovered collimator design based on simulation. The contour displays the energy of the thermal neutron from the beginning of collimator until the aperture. The red region in the plots indicates the highest energy flux while the blue area indicates low energy flux.

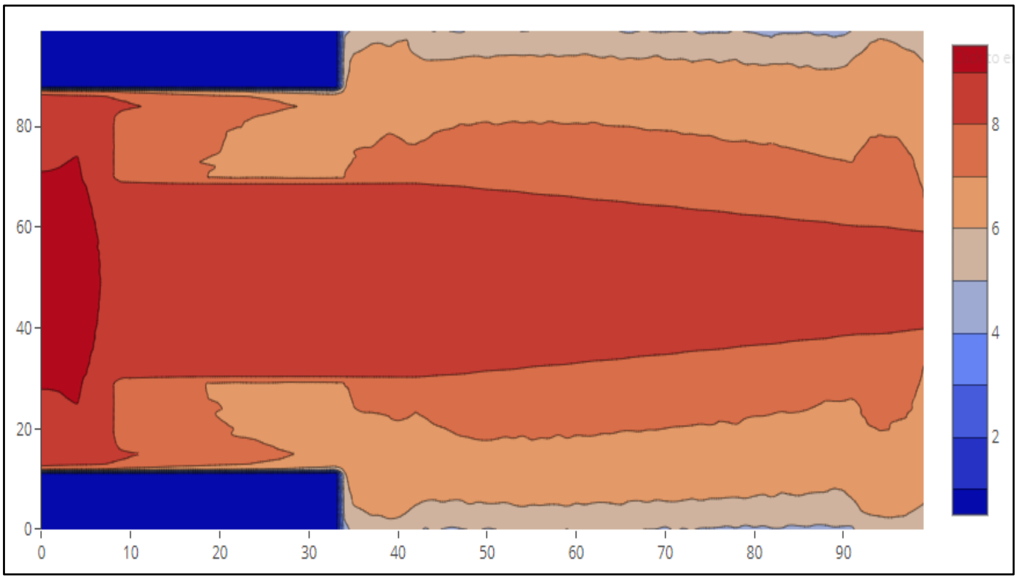

Figure 8. Contour plot of thermal neutron from uncovered collimator using MCNPX.

The contour shows that the high energy flux from the source had to lose their energy along the distance [9]. At the 10 cm of the collimator, the flux energy had started losing their energy. The thermal neutron flux show collimates and maintains the energy from the 10 cm to end of the collimator. This result verifies the uncovered collimator is sufficient in keeping the neutron on collimator compared to the fully covered collimator. Based on the selection, an ideal collimator finalized with using the material and shielding thickness from design D1, the size of the aperture of 3cm and use an uncovered collimator structure. The next step taken of this research is to compare the simulation result of the collimator and preliminary measurement using gold foil activation analysis in earlier data. Figure 9 shows the geometry of the finalized BNCT collimator at the thermal column using MCNP.

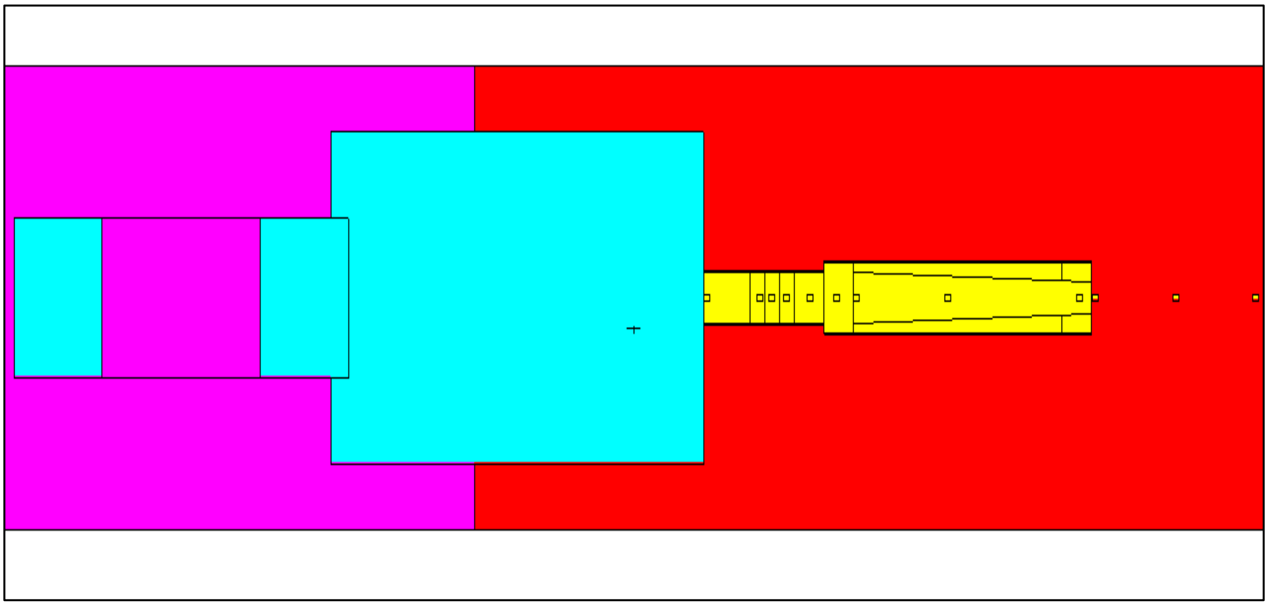

Figure 9. The illustration of collimator at the thermal column of RTP using MCNPX.

3.2. Collimator performance

To construct the validity of the collimator performance, the simulation result using MCNPX was compared to the experimental result from gold foil activation analysis. The result compared to the thermal and epithermal neutron flux produced along the thermal column at Phase1, Phase 2 and Phase 3 of the thermal column at 250kw of RTP power. In preliminary measurement using gold foil activation analysis, there is no collimator, but in the simulation, the collimator located at Phase 2 [10]. Figure 10 display the thermal neutron flux along the thermal column with and without collimator on Phase 2. The presence of collimator at Phase 2 of the thermal column had better thermal neutron production rather than without the collimator install. At the distance 142 cm or the initiation of Phase 2, the experiment shows that the thermal neutron flux was a drop from the 10^{10} neutron.cm^{-2}s^{-1} to 10^{7} neutron.cm^{-2}s^{-1} but with the presence of collimator, the thermal neutron flux was slightly lower within the range of 10^{8} neutron.cm^{-2}s^{-1}. The collimator was sustained the thermal neutron flux until at the 283.9 cm with only 20% of thermal neutron reduced. On other hands, from Phase 2 to Phase 3 without the collimator, an experiment was measured that the thermal neutron reduced to 96%. Overall, the thermal neutron with the collimator installation can sustain the higher thermal neutron flux from the RTP that can be used for BNCT research.

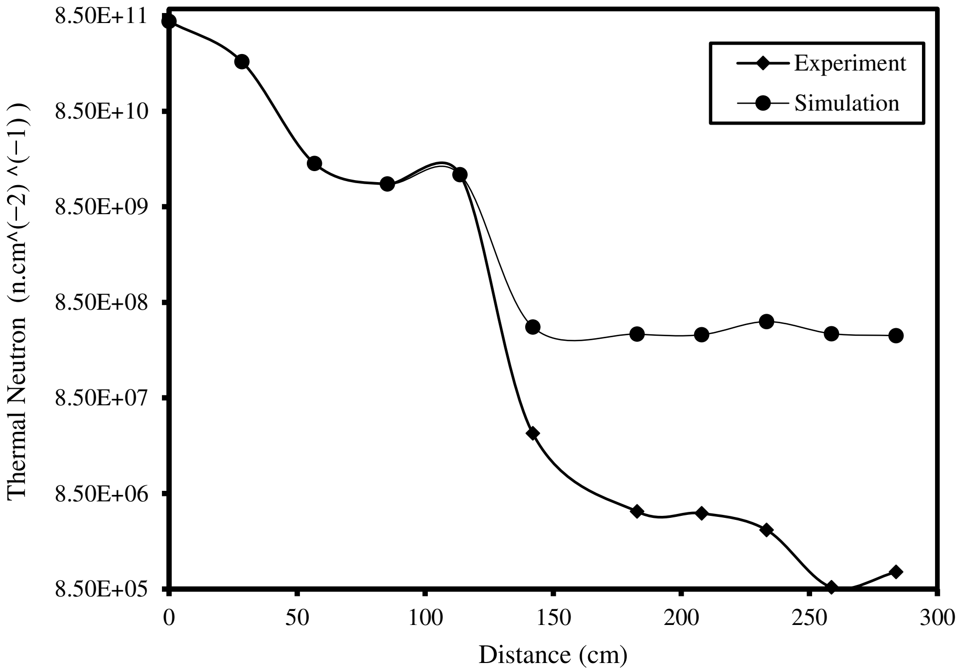

Figure 10. The graphical different of thermal neutron flux along the thermal column by simulation (collimator) and experiment.

The simulation of epithermal neutron flux produced also shows the same trend as thermal neutron flux on figure 11. The existence of collimator conserved the epithermal neutron with only less than 40% loss of the epithermal neutron flux. In contrast, the particle loss from Phase 2 to the Phase 3 was almost 99% due to particle loss on air. The material use inside the collimator was functioned to prevent too many particle losses along though the distance and keep maintaining the epithermal flux to be used for BNCT research. Even though the aperture size without collimator was 25 cm, but the number of epithermal neutrons is still low and keep decreasing tremendously as the distance increase.

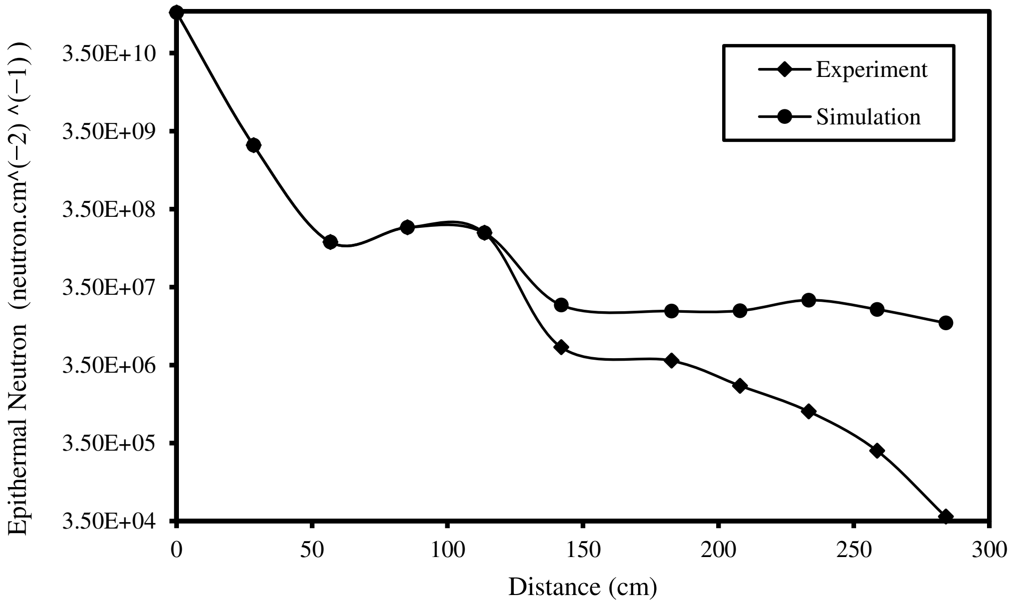

Figure 11. The graphical different of epithermal neutron flux along the thermal column by simulation (collimator) and experiment.

The comparison between the simulation and experimental show the concrete validity of the thermal neutron and epithermal neutron beam can be sustained and use for BNCT if the collimator were installed at the Phase 2 of the thermal column. Even tough with 250kW of RTP power the thermal neutron was insufficient enough for BNCT clinical trials, but the beam was sufficient for research and development for BNCT with extended period of time. The clinical trials of BNCT required 1.0 x 10^9 neutron.$cm^{-2}s^{-1}$ for 30 minutes of treatments, but with the 3.28 x 10^8 neutron.$cm^{-2}s^{-1}$ of thermal neutron estimated it can be used for almost 1-2 hour for BNCT clinical research [9]. At 300kW of RTP power, the thermal neutron flux was believed to be more than standard BNCT requirement but the safety and shielding must be first priority.

4. Conclusion

Simulation result from MCPNX shows that the ideal collimator was selected based on the uncovered and fully covered collimator structure. The collimator design D1 with the uncovered structured was chosen for BNCT collimator application the simulation of ideal collimator produces 3.82 x 108 neutron.cm-2s-1 for thermal neutron and 1.21 x 107 neutron.cm-2s-1 for epithermal neutron and the result was then compared with the preliminary measurement of neutron along the thermal column on Phase 1, Phase 2, and Phase 3. The used of the ideal collimator based on D1 design have optimized the beam by increase the thermal neutron and the epithermal neutron at the end of collimator compared to without using the collimator. Therefore, the use of MCNP simulation software is important in order to study and design for the nuclear application such as BNCT facility.

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