Monte Carlo simulation for designing collimator of neutron diffractometer facility in Malaysia

Muhammad Aliff Ashraff Rosdi¹, Pei Sean Goh¹,a), Safwan Shalbi¹, Faridah Idris², Rafhayudi Jamro², Norriza Mohd Isa²

¹Nuclear Engineering Department, School of Chemical and Energy Engineering, Faculty of Engineering, University Teknologi Malaysia, 81310 Skudai, Johor Bahru, Malaysia.
²Malaysia Nuclear Agency, 43000 Kajang, Selangor, Malaysia

a)peisean@petroleum.utm.my

Abstract. Neutron diffraction (ND) is an application of non-destructive test which involves the process of interference between neutron and atoms within materials. This technique has drawn many attentions especially in industrial, metallurgical and nuclear sectors. Neutron diffractometer system (NDS) is a system which includes all the instrumentation to perform ND technique. One of the most important instruments in NDS set-up is neutron collimator which is used to reduce the size and steer the direction of the beam. Generally, neutron collimator used in NDS is based on step convergent collimator type. Currently, the NDS facility is planned to be built at one of the radial beam port of TRIGA MARK II PUSPATI research reactor (RTP) in Malaysia. The aim of this research is to characterize the materials suitable for neutron collimator and to obtain the ideal geometry for neutron collimator design. In order to achieve these aims, several neutron collimators with different geometries have been designed using Monte Carlo Simulation Codes MCNPX. The results are then compared to obtain the best design with high thermal neutron flux and low gamma contamination at the object plane. This research may be useful in the selection of neutron collimator design for NDS facility at TRIGA research reactor.

1. Introduction
Reactor TRIGA PUSPATI (RTP) is a pool type light water research reactor using enriched uranium zirconium hydride (UZrH₁₆) fuel with enrichment of 19.9% U²³⁵ and is located in Malaysia. RTP has a nominal thermal power of 1MW with maximum brilliance of 1.897x10¹³ neutrons cm⁻²s⁻¹ obtained at 750kW [1]. RTP is composed of a thermal column and four neutron beam ports including three radial and one tangential beam ports as illustrated in Figure 1. Since its first commissioning in June 1982, various research works have been conducted using the neutrons produced from the RTP. However, until now, only two of the existing beam ports were used which are beam port 3 for neutron radiography (NR) and beam port 4 for small angle neutron scattering (SANS). In order to maximize the utilization of beam port facility of RTP, previous researches claimed that NDS can be developed at radial beam port 1 [2].
Neutron diffraction (ND) is one of the neutron scattering applications which has been widely used to determine atomic structure of material, measuring strain within material and study the composition of crystal and amorphous materials. In order to implement ND technique, thermal neutron with intensity at least $10^4$ neutron cm$^{-2}$s$^{-1}$ is necessary [2]. Besides, the size and operational condition of the system need to be optimized and properly shielded by following diffraction rules and regulations. Generally, neutron diffractometer system (NDS) consists of several vital instrumentations including collimator. Neutron collimator is a beam forming assembly where function is to reduce the cross section of neutron beams and to align the direction of neutron beams in a specific direction. Basically, neutron collimator contains the assembly of gamma and fast neutron absorbing plates in order to filter the contaminations. Neutron collimator is composed of the combination of neutron and gamma absorber materials such as borated paraffin, cadmium, borated polyethylene, indium, gadolinium oxide, boron-aluminium plate, lead and bismuth to shield neutron and gamma particles respectively. Neutron collimator utilized in Romanian research reactor was constructed using boron-aluminium plate, indium and lead materials while collimator in HANARO research reactor in South Korea is composed of boron-based materials and bismuth [4][5]. Besides, GGR-1 research reactor located in Greece uses the neutron collimator fabricated from the assembly of borated polyethylene, lead, and Mylar films coated with gadolinium oxide [6]. Researchers from China proposed a collimator design consisted of bismuth, series of leads and boron based materials [7]. In addition, placement of sapphire crystal in the collimator is highly recommended as it has strong attenuation coefficient toward epithermal and fast neutrons while low attenuation coefficient toward thermal neutrons [8]. Selection of neutron collimator geometry for ND technique needs to be emphasized based on the uniformity and maximum flux produced at the end of the collimator outlet.

In this study, Monte Carlo MCNPX code is used to obtain the most optimal neutron collimator geometry for neutron diffractometer system with respect to neutron and gamma radiation. Several collimators with different combination of neutron and gamma absorbent materials were designed and tested in order to obtain the ideal thermal neutron flux at the end of the collimator tube. The findings of this study may be useful to the development of neutron collimator design combining neutron and gamma shielding materials.

2. Methodology

Calculation of radiation transport and dosimetry inside the neutron diffractometer collimator was performed using the Monte Carlo MCNPX code. The neutron collimator for NDS facility has an overall length of 166cm with two sections as shown in Figure 2. The collimator is divided into two parts, first part has a diameter of 18cm with length of 50cm, and second part has a diameter of 20cm with length of 115cm. There are an additional length of 1cm extra with diameter of 24cm on the second part of collimator which functions as step to ease the handling of neutron collimator. Basically, material used for the exterior part of neutron collimator is made from aluminium as it is a low activation element as compared to steel. Furthermore, the neutron collimator was coated with lead and boron flex in order to reduce scattering of neutron and gamma radiations.
Figure 2: External design of neutron diffractometer collimator.

The main purpose of this research is to design and simulate several step convergent collimator in order to achieve high thermal neutron flux and low gamma contamination. Step convergent collimator type is chosen in order to produce small size of thermal neutron beam. This is because beam from neutron diffractometer collimator should be sharp to allow the investigation of specific location on object. The characteristic of an ideal neutron beam are parallel, higher flux intensity, mono-energetic, uniform cross-section, and lower contamination of unwanted radiations [9]. In this study, a total of 8 designs of neutron collimator with different materials selection and geometry were investigated. Arrangement and position of the materials were made inside of the collimator. The following materials in Table 1 were used: high density polyethylene (HDPE), bismuth, lead, borated paraffin, borated polyethylene and sapphire crystal. Geometry of the materials is shown in Figure 3 and Table 2.

| Material   | Neutron attenuation coefficient | Gamma attenuation coefficient | Description          |
|------------|---------------------------------|------------------------------|----------------------|
| 5% BPF     | 2.35                            | 0.14                         | Neutron shielding    |
| 5% BPE     | 2.36                            | 0.14                         |                      |
| 30% BPE    | 2.68                            | 0.17                         |                      |
| HDPE       | 0.63                            | 0.15                         |                      |
| Lead       | 0.26                            | 3.00                         | Gamma shielding      |
| Bismuth    | 0.19                            | 2.98                         |                      |
| Sapphire   | 0.24                            | 0.76                         | Fixed               |

Table 2. Material geometry of neutron diffractometer collimator.

| No. of collimator | Material                                      |
|-------------------|-----------------------------------------------|
| A                 | 5% borated paraffin + lead + sapphire        |
| B                 | 5% borated paraffin + bismuth + sapphire     |
| C                 | High density polyethylene + lead + sapphire  |
| D                 | High density polyethylene + bismuth + sapphire|
| E                 | 5% borated polyethylene + lead + sapphire    |
| F                 | 5% borated polyethylene + bismuth + sapphire |
| G                 | 30% borated polyethylene + lead + sapphire   |
| H                 | 30% borated polyethylene + bismuth + sapphire|
3. Results and discussions

The results obtained from MCNPX calculations at the centre and outer part of collimator tube were shown in Figure 4 and Figure 5.

Figure 4 shows that average thermal neutron flux produced at the centre of the collimator was $6.23 \times 10^6$ neutron cm$^{-2}$s$^{-1}$, fast neutron flux was $2.03 \times 10^5$ neutron cm$^{-2}$s$^{-1}$ and gamma flux was $1.20 \times 10^1$ γ cm$^{-2}$s$^{-1}$. The highest thermal neutron flux was obtained at centre part of collimator C with flux of $6.32 \times 10^6$ neutron cm$^{-2}$s$^{-1}$ which is consisted of HDPE and lead material. On the other hand, the lowest thermal neutron flux was measured at collimator B which consisted of 5% BPF and bismuth material.

Thermal neutron flux was high when lead is used instead of bismuth. This is because lead can also moderate fast neutron which indirectly increases intensity of thermal neutrons in the collimator. In addition, lead also has high scattering cross section properties that cause the neutrons to scatter inside of the collimator [10]. In case of fast neutron flux, most of the collimator yields high intensity of fast neutron at the centre region. Therefore, this does not rank so high in the design selection. Furthermore, the fast neutron flux produced in the collimator could be useful in order to increase the intensity of thermal neutron flux by moderation. Besides, based on Figure 3, collimator with bismuth and lead materials give an equivalent result of gamma absorption at the low average of $10^1$ γ cm$^{-2}$s$^{-1}$. The reason is that bismuth and lead has high gamma absorption cross section [11]. Even though the
gamma radiations are still present in the collimator, the average gamma flux yielded from the centre region of the collimator were considerably low for bismuth and lead [12].

According to Figure 5, the average neutron flux and gamma flux measured at the end of outer region were lower compared to centre region. This is because the ionising radiations produced from the reactor core directly interacted with the shielding materials at the outer region compared to the centre region of collimator. The average of thermal neutron and fast neutron fluxes yielded at the end window were $3.74 \times 10^3$ neutron cm$^2$s$^{-1}$ and $8.29 \times 10^2$ neutron cm$^2$s$^{-1}$, respectively. The lowest thermal neutron flux was obtained at collimator H which consist of 30% BPE and bismuth while the lowest fast neutron flux was obtained at collimator C of HDPE and lead. However, the results of neutron
fluxes obtained for all collimator design were better which is 99% lower than the fluxes yielded at the centre region. The reason is most of the neutron particles have been absorbed by the neutron shielding materials in the collimator. In case of gamma flux, no flux was simulated at the outer region of the collimator. This implies all of the incident gamma radiations have been totally absorbed by the shielding materials in the collimator. This also proved that both lead and bismuth material are very excellent gamma absorber.

Figure 5 also shows that collimator implemented with bismuth yields more intensity of fast neutrons compared to lead. This shows that while bismuth and lead are very good against gamma shielding, their shielding properties of fast neutron were different. This is because bismuth is more transparent against fast neutron while lead is able to thermalize fast neutron indirectly which substantially reduce intensity of fast neutron. According to Figure 5, direct interaction of neutron particles with these shielding materials causes the production of secondary gamma radiation. The production of secondary gamma radiation was highest at collimator implemented with HDPE material. In case of the other designs which consist of boronated materials, the production of secondary gamma radiation was 87% lower than collimator with HDPE material.

After all the results have been compared, collimator E which composed of 5% BPE and lead material was selected [Figure 6]. This is because of the production of secondary gamma radiation obtained from the neutrons interaction is the lowest compared to the other collimator designs. The emergence of this secondary gamma radiation was not desirable since it may cause harm to the sample and other instrumentations of NDS [2]. Besides, the production of thermal neutron was high in the centre region of the collimator. The high intensity of thermal flux at the window end of the collimator is required since it is one of the most vital criteria of a NDS facility. The fast neutron yielded from the collimator E was also acceptable as the intensity was about average with the other collimator designs. Lastly, there is no gamma radiation at the outer region and some low level of gamma at the centre region of collimator.

![Figure 6. Final design of collimator.](image)

4. Conclusion
The characterization of suitable materials for collimator used in NDS has been simulated using the MCNPX code. Collimator E which composed of 5% borated polyethylene and lead has been selected as the ideal design of collimator for NDS at RTP. The results obtained from this paper may be useful for the construction of new neutron diffraction system facility at TRIGA research reactor.

5. References
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