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Design of Moderator Neutron for Boron Neutron Capture Therapy in Kartini Nuclear Reactor Using Monte Carlo N Particle 5 Simulation

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Abstract. The optimation of moderator design on radial piercing beam port in Kartini Nuclear Reactor using MCNP5 simulation has been carried out. This optimation has been used for obtaining neutron flux according to International Atomic Energy Agency (IAEA) regulation. The methode used in this experiment was combination of shifting methode and filtering methode. Independent variables varied, were material and thickness of collimator wall, moderator, filter and gamma shielding. Optimized epithermal neutron flux of the collimator for BNCT has been achieved 1.20×10^{9} n/cm^{2}s. The result of beam quality are 0.8 for neutron current component, 0.03 for thermal neutron component, 312×10^{-13} Gy cm^{2}s/n for fast neutron component and 38.5×10^{-13} Gy cm^{2}s/n for gamma contamination component. It can be concluded that, the designed moderator is feasible and applicable for BNCT.

1. Introduction

According to GLOBOCAN 2012, an estimated 14.1 million new cancer cases and 8.2 million cancer-related deaths occured in 2012, compared with 12.7 million and 7.6 million, respectively, in 2008. Prevalence estimates for 2012 show that there were 32.6 million people (over the age of 15 years) alive who had had a cancer diagnosed in the previous five years [1].

There are several kinds of treatment to cure the disease or considerably prolong life while improving the patient's quality of life. Those treatments are, generally, sorted into 3 majors: surgery, radiotherapy, and systemic therapy [2]. Radiotherapy is a common cancer treatment that uses high doses of radiation to destroy cancer cells and shrink tumours. X-rays, γ-rays, and charged particles are types of radiation used for cancer treatment. These radiations used in high level of energy, thus they may cause ionizations in the surrounding normal cells [3,4].

Boron Neutron Capture Therapy (BNCT) is another form of radiotherapy. In BNCT, ^{10}B and its carrier drug are administered to the patient. This carrier will take these compounds to the location of the tumour cells, where ^{10}B is supposed to be accumulated. On the next step, the tumour area is to be irradiated by neutron beam. There are two different neutron beams commonly used in BNCT: thermal neutron beam for superficial tumours and epithermal neutron beam which may penetrate to relatively deeper locations (8 cm to 10 cm depths). Theoretically, an epithermal neutron becomes a thermal neutron when it reaches the tumour

cells after undergoes moderations by materials (especially water) contained in the human's body along its path. Then, ^{10}B in the tumour cells captures the thermal neutron, resulting in a prompt nuclear reaction ^{10}B(n,α)^{7}Li [5]. Both α-particle and the fission fragment ^{7}Li have high LET characteristics (175 keV.μm^{-1} and above) and short path lengths (approximately 4.5 to 10 μm), hence the energy deposition is locally limited around the tumour cells [4].
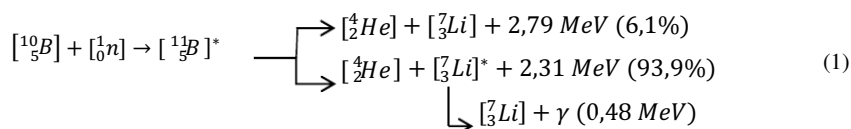
In Indonesia nowadays, three research reactors are available, all are operated by the National Nuclear Energy Agency (BATAN). Those reactors are TRIGA 2000 reactor in Bandung, TRIGA MARK-II reactor in Yogyakarta, and Multipurpose Research Reactor in Serpong. Of these three reactors exist, only TRIGA reactors are planned to be added with a facility for BNCT purpose. Any BNCT facility has not been established yet; feasibility study is still in its process, indeed. In TRIGA MARK-II type research reactor in Yogyakarta, which has also been known as Kartini Research Reactor, the facility for BNCT is going to be built for an advanced study which uses tumour-injected animals as the object [6].

Kartini Research Reactor has an operational output thermal power of 100 kW. The radial piercing beam port of this reactor is planned to be implanted with a device which is capable of narrowing the neutron beam, called as moderator. Radial piercing beam port is selected since it is the most flexible part of the reactor which could be modified. Due to the tendency of epithermal neutron beams usage for BNCT, the moderator must contains materials needed to produce an epithermal neutron beam which fulfill some particular characteristics. Thus, a proper moderator has to be designed so that the output neutron beam reaches criteria recommended by the International Atomic Energy Agency (IAEA).

2. Theory

2.1 Boron neutron capture therapy (BNCT)

Boron neutron capture therapy (BNCT) is based on the nuclear capture and fission reactions that occur when ^{10}B, which is a non-radioactive constituent of natural elemental boron, is irradiated with low energy (0.025 eV) thermal neutrons. This results in the production of high linear energy transfer (LET) alpha particles ^{4}He and recoiling ^{7}Li nuclei, as shown below [4].

$$\left[{}^{10}_{5}B\right] + \left[{}^{1}_{0}n\right] \rightarrow \left[{}^{11}_{5}B\right]^{*} \begin{cases} \left[{}^{4}_{2}He\right] + \left[{}^{7}_{3}Li\right] + 2{,}79\ MeV\ (6{,}1\%) \\ \left[{}^{4}_{2}He\right] + \left[{}^{7}_{3}Li\right]^{*} + 2{,}31\ MeV\ (93{,}9\%) \\ \qquad \downarrow \left[{}^{7}_{3}Li\right] + \gamma\ (0{,}48\ MeV) \end{cases} \qquad (1)$$

In order for BNCT to be successful, a sufficient amount of ^{10}B must be selectively delivered to the tumor (~20 μg/g or atoms cell), and enough thermal neutrons must be absorbed by them to sustain a lethal ^{10}B(n, α)^{7}Li capture reaction. Because the high LET particles have limited path lengths in tissue (5-9 μm), the destructive effects of these high-energy particles are limited to boron containing cells [4].

2.2 Desired neutron beam parameters

Epithermal neutron beam entering tissue creates radiation field with a maximum thermal flux at a depth 2 to 3 cm, which drops exponentially thereafter. In contrast to the epithermal beam which shows a skin-sparing effect, the thermal flux falls off exponentially from the surface. Thus, thermal neutron irradiations have been used for tumour treatments in the skin. In

general, however, the current trend for treatment of patients is using epithermal neutron beams [7].

The main collimator designing objective is to deliver an epithermal neutron beam within a reasonable treatment time and to produce the desired thermal neutrons at tumour depth with minimal other radiations present. The two principal beam characteristic of interest are intensity and quality. Beam intensity will be the main determinant of treatment time. Beam quality relates to the types, energies, and relative intensities of all the radiations present [7].

2.2.1 Epithermal Beam Intensity. For the purposes of reporting beam intensity, the common definition for an epithermal energy range should be used, namely 0.5 eV to 10 keV. Current experience shows that desirable minimum epithermal neutron beam intensity would be 10^9 $n.cm^{-2}.s^{-1}$. Beam of $5 \times 10^8 n.cm^{-2}.s^{-1}$ are usable, but result in rather long irradiation times. Where there is a choice to be made, most practitioners would rather have better quality rather than more intensity [7].

2.2.2 Incident Beam Quality. Beam quality is determined by four parameters under free beam conditions. They are discussed below in order of importance [7].

1. The fast neutron component
   In BNCT the energy range for fast neutrons is taken as > 10 keV. Fast neutrons, which accompany the incident beam, have a number of undesirable characteristics such as free radicals production. Therefore, it is one of the main objectives of BNCT beam design to reduce the fast neutron component. In existing facilities, the range of dose from this component is from 2.5 to 13×10^{-13} $Gy.cm^2$ per epithermal neutron, meanwhile the target number should be 2×10^{-13} $Gy.cm^2$ per epithermal neutron[7].

2. The γ-ray component
   It is desirable to remove γ-ray radiation from the beam. A target number for this should be 2×10^{-13} $Gy.cm^2$ per epithermal neutron. The range in existing facilities is from 1 to 13×10^{-13} $Gy.cm^2$ per epithermal neutron[7].

3. The ratio between the thermal flux and the epithermal flux
   To reduce damage to the scalp, thermal neutrons in the incident beam should be minimized. A target number for the ratio of thermal flux to epithermal flux should be 0.05[7].

4. The ratio between the total neutron current and the total neutron flux
   This ratio provides a measure of the fraction of neutrons that are moving in the forward beam direction. A high value is important for two reasons; to limit divergence of the neutron beam (thereby, reduce undesired irradiation of other tissues) and to permit flexibility in patient positioning along the beam central axis. A target number for this ratio should be greater than 0.7[7].

2.3 Neutron source for BNCT

Several experiences in designing collimator for BNCT have been conducted both based on the materials selection and the geometry optimizing. A collimator at least consists of 5 components: collimator wall, moderator, filter, γ-ray shielding, and aperture. Hereby, explained each of those parts.

2.3.1. Collimator wall. Collimator wall should reflect neutrons back into the inner part of collimator. Therefore, neutron reflecting type material is used. Suitable reflector materials for this are those with high scattering cross section and high atomic mass (resulting in little energy loss). They include Pb, Bi, PbF_2 [7]. In his experiment, Marko Maučec found Ni outperformed other materials, Pb, Bi and PbF_2, with the highest epithermal neutron flux as the result, also made a collimator design with Kyviv Research Reactor as the neutrons source. In their study they used Ni as collimator wall layer. From this study they got that the epithermal neutron flux grew up as the Ni layer became thicker up to 6.5 cm, then it started to fall off slowly [7,8]. Walls that are used near the beam exit are beam delimiters and it should absorb rather than reflect neutrons. This part is made of B_4C or $^6Li_2CO_3$ dispersed in polyethylene. Epithermal neutrons striking the wall of the collimator are thermalized and captured. It should be noted that ^{10}B emits a low energy capture γ-ray (478 keV) but ^6Li does not and its use is to be preferred in locations close to the patient [7].

2.3.2. Moderator. Moderation of fast neutrons is best accomplished by low atomic mass materials. Any moderator or filter materials chosen must not decompose in a high radiation field, nor produce moisture. Any neutron activation products from the materials should be short lived. Some suitable candidates that widely used are Al, Al_2O_3, and AlF_3. Combinations of Al followed by Al_2O_3 or AlF_3 downstream are very efficient because the O and F cross-sections fill in the valleys between the energy resonance peaks of Al [7].

2.3.3. Gamma-ray shielding. Materials such as Pb and Bi may be placed in the beam to reduce γ-rays originating from the reactor core, but these will nonetheless reduce neutron beam intensity. Bi is nearly as good as Pb for shielding γ-rays, while having a higher transmission of epithermal neutrons [7].

2.3.4. Filter. The objective is to filter out all neutrons but the epithermal neutrons from the reactor beam. For epithermal neutron beams, it is desirable to limit thermal neutron contamination by filtering. Filter materials for thermal neutrons require either elements with ^6Li, ^{10}B or Cd. Cd is most frequently used absorber due to the reason that Cd is an effective (n,γ) converter [7]. Not only thermal neutrons, but also fast neutrons are very necessary to reduce. This can be done with natural or isotopically enriched materials, for which an interference minimum in the total neutron cross section exists in epithermal energy range. The total cross section of ^{60}Ni isotope has the deep and wide interference minimum in the energy range from several eV to 10 keV and therefore this material is useful for BNCT purposes [7].

2.3.5. Aperture. Aperture is a part of collimator which provides required cross section of the beam. Because of its role in the collimator, it is often found to be located at the end point of collimator. In this study, the collimator which is going to be built is for trials with 1 to 2 cm sized tumor cell samples and tumor-injected animals as the object. For the tumor-injected animals, the size of tumor cells would be monitored. Once the tumor reaches the detectable size, it would be irradiated immediately. Hence the minimum detectable size of tumor should be known. James Michaelson used screening mammography to detect breast tumor. According to the result of the study, it was found that the median size at which breast tumors

become operationally detectable by screening mammography was approximately 7.5 mm, with relative efficiency of 50%. A higher relative efficiency of 80% appeared for 10 mm tumor detection, and 100% for 30 mm tumor detection [9].

2.4 The monte carlo method and mcnp program

The Monte Carlo method can be used to duplicate theoretically a statistical process (such as the interaction of nuclear particles with materials). The individual probabilistic events that comprise a process are simulated sequentially.
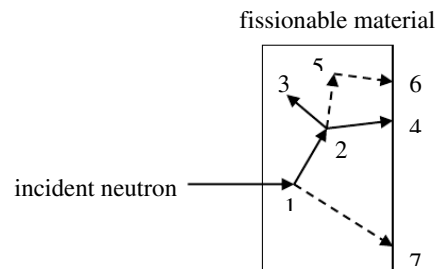
fissionable material

Figure 1. Random history of a neutron incident on a fissionable material slab [10].

The probability distributions governing these events are statistically sampled to describe the total phenomenon. The statistical sampling process is based on the selection of random numbers based on the physics rules and probabilities governing the processes and materials involved [10]. Figure 1 depicts a random history of a single neutron incident on a slab of material that can undergo fission reaction. Numbers between 0 and 1 are selected randomly to determine what and where interaction takes place In this particular example, a neutron collision occurs at event 1. The neutron is scattered in the direction shown. A photon is also produced and is temporarily stored (*banked*) for later analysis. At event 2, fission occurs, resulting in the termination of the incoming neutron and the birth of 2 outgoing neutrons and 1 photon. The neutron and the photon are banked for later analysis. The first fission neutron is captured at event 3 and terminated. The banked neutron is now retrieved and leaks out of the slab at event 4. The fission-produced photon has a collision at event 5 and leaks out at event 6. The remaining photon generated at event 1 is now followed with a capture at event 7. This is a quite satisfying example of random phenomena generated in the Monte Carlo method. As more and more such histories are followed, the neutron and photon distributions become better known[10].

3. Methods

3.1 Material

This study was a simulation-basic experiment. Materials used are listed as personal computer, MCNP5©software, notepad, comand promt, Microsoft Office Word© 2010 and Microsoft Office Excel© 2010. Monte Carlo N-Particle version 5 (MCNP5) was used for the simulations of phenomena of interest. MCNP was a general-purpose Monte Carlo N-Particle code that can be used for neutron, photon, electron, or coupled neutron/photon/electron transports.

Specific areas of application include, but were not limited to, radiation protection and dosimetry, radiography, medical physics, nuclear criticality safety, and also fission and fusion reactor design. MCNP5 was the latest version of MCNP which included some additions of photonuclear database, superimposed mesh tallies and time splitting ability. Meanwhile, MCNP6 was still being developed.

3.2 Kartini research reactor modelling
Kartini Research Reactor specifications are documented in the Safety Analysis Report (SAR) of the reactor. It was needed to make a model of the reactor since it would be used as the neutrons source. An MCNP input file is divided into 3 main blocks (which are known as *cards*) so called cell cards, surface cards, and data cards. The first two cards correspond to the geometry definition, while the data cards contain all the information related to the specification of the particle source, the definition of the materials, and the tallies. By using these codes, Kartini Research Reactor was modelled, as the first step.
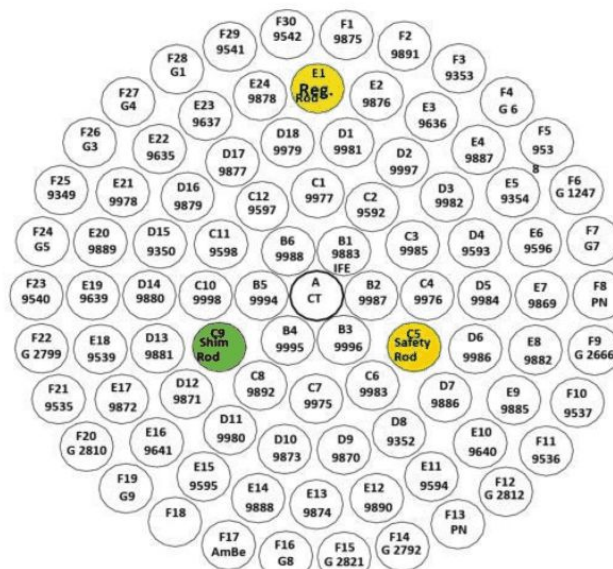

Figure 2. Core Configuration.

Kartini Research Reactor is a TRIGA MARK-II research reactor type. It has a maximum thermal power of 250 kW. The reactor was modelled by using MCNP5 program with core configuration as depicted in Figure 2. Several other parts of the reactor, whose existence were considered to affect to the reactor criticality, were also modelled, such as the radial reflector, rotary specimen rack, and piercing beam port. Moreover, the radial piercing beam port was also built since it would become the point of interest; where the collimator would be built.

3.3 Data variable
The beam criteria suggested by the IAEA, as shown in Table 1 below.

Table 1. Beam parameters.

Parameter	Nomenclature
Epithermal beam intensity	Φ_{epi} (n.cm^{-2}.s^{-1})
Fast neutron dose per epithermal neutron	D_f / Φ_{epi} (Gy.cm^2.n^{-1})
Gamma dose per epithermal neutron	$\dot{D}_\gamma / \Phi_{epi}$ (Gy.cm^2.n^{-1})
Ratio between thermal flux and epithermal flux	Φ_{th} / Φ_{epi}
Ratio between neutron current and neutron flux	J / Φ_{epi}

It was said in the IAEA's technical document that most practitioners would rather have better quality of the neutron beam than more intensity. It was also emphasised that the beam quality was determined by four parameters, in order of importance: fast neutron component, γ-ray component, thermal neutron component, and directionality. Thus, the designing process was done according to this rule. Table 2 shows the desired BNCT-purpose beam in this study.

Table 2. Beam criteria.

Nomenclature	Value
Φ_{epi} (n.cm^{-2}.s^{-1})	$> 1.0 \times 10^9$
D_f / Φ_{epi} (Gy.cm^2.n^{-1})	$< 2.0 \times 10^{-13}$
$\dot{D}_\gamma / \Phi_{epi}$ (Gy.cm^2.n^{-1})	$< 2.0 \times 10^{-13}$
Φ_{th} / Φ_{epi}	< 0.05
J / Φ_{epi}	> 0.7

4. Results and discussion

4.1 Reactor Criticality
The criticality calculation by using MCNP5 gave result 1.0050 ± 0.0004, which was a good approach to the criticality value of 1.000 ± 0.010. The thermal neutron flux in Ring F of the reactor core was $1,12 \times 10^{12}$ n.cm^{-2}.s^{-1}, mean while the real value, which was detected by a study, was approximately $1,12 \times 10^{12}$ n.cm^{-2}.s^{-1}. This same might be caused by the multiplication factor inputted into the MCNP5 codes was $1,883 \times 10^{16}$ n.s^1. With these results, collimator designing was then conducted.

4.2 Collimator Wall
Natural nickel is a very good material to be employed as a neutron collimator wall. Its atomic mass which is not too small, that would make too much energy decrement of neutrons, and yet not too high, that only would slightly shift the energy spectrum of neutrons. Hence without moderator, the natural nickel itself already produce epithermal neutron-dominated

beam, but still needs more materials to raise its quality. The results of simulation for wall thickness variation are depicted in Figure 3.
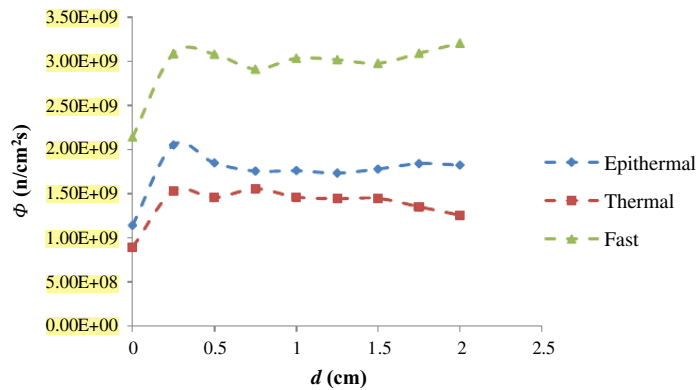

Figure 3. Epithermal neutron flux for various thickness of wall Ni-nat.

4.3 Moderator

The simulations proved that ^{32}S outperform the other materials, as depicted by the Figure 4. For a comparison, with Al, AlF$_3$, and Al$_2$O$_3$, ^{32}S produced epithermal neutron flux higher than them. Thus ^{32}S was chosen as material for moderator.
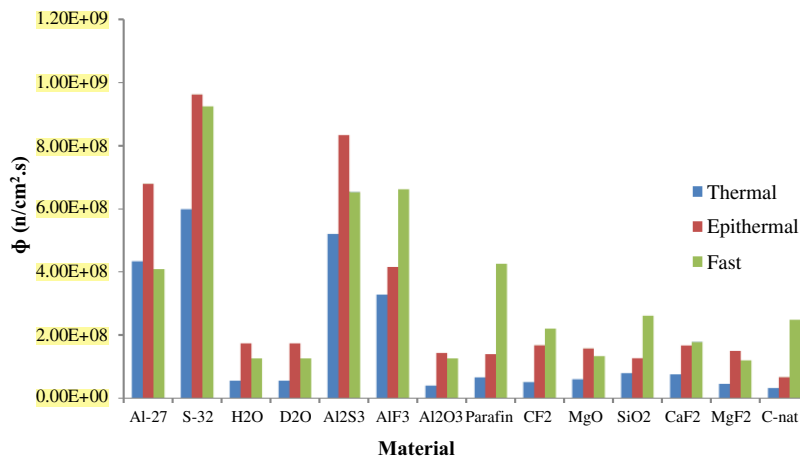

Figure 4. Comparison of moderator materials.

4.4 Filter
Figure 4.3 depicts that the comparison of filter materials.1mm thick of filter is actually enough to decrease the thermal neutron component to 0.03, which is far below the recommended maximum value, 0.05.
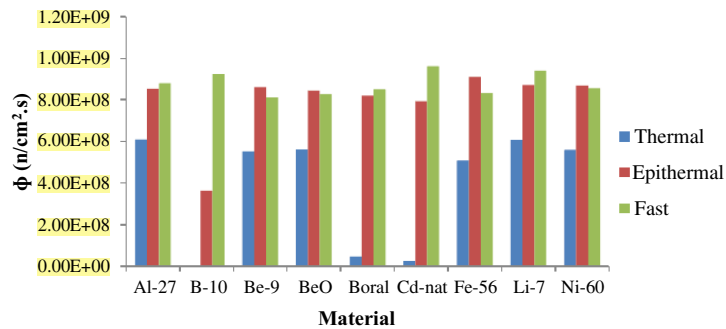

Figure 5. Comparison of filter materials.

4.5 Gamma-ray shielding
The γ-ray component is reduced exponentially by using Bi. With thickness of 7 cm, the γ-ray component remains 2.454×10^{-13} Gy.cm^2.n^{-1}. The addition for more thickness will, of course, decrease the γ-ray component. Unfortunately, as Bi made thicker, the fast neutron component increases, as shown in Figure 6.
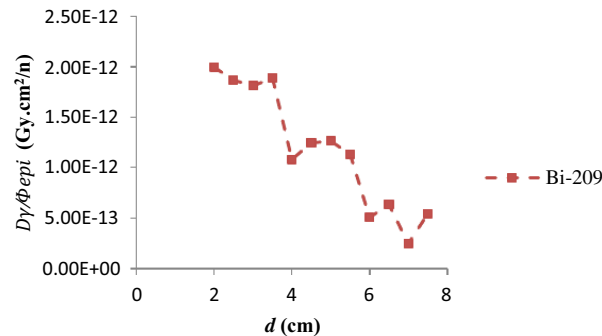

Figure 6. Gamma-ray component for various thickness of shielding ^{209}Bi.

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4.6. Final result of collimator conceptual design

Table 5. Final result of beam characteristic.

Design	Φ_{epi} (n/cm^{2}s)	J/Φ_{total}	Φ_{th}/Φ_{epi}	D_f/Φ_{epi} (Gy cm^2/n)	D_γ/Φ_{epi} (Gy cm^2/n)
I	$1{,}20 \times 10^9$	0,8	0,03	312×10^{-13}	$38{,}5 \times 10^{-13}$
II	$0{,}06 \times 10^9$	0,7	0,04	41×10^{-13}	$1{,}27 \times 10^{-13}$
III	$0{,}76 \times 10^9$	0,543	0,03	158×10^{-13}	$2{,}45 \times 10^{-13}$

The figure of collimator conceptual design:
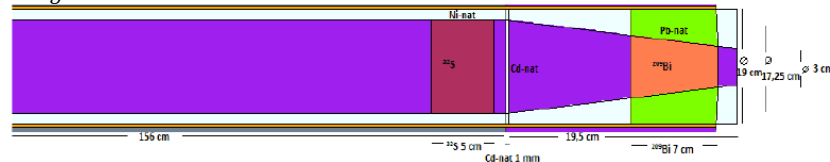
4.6.1. Design I

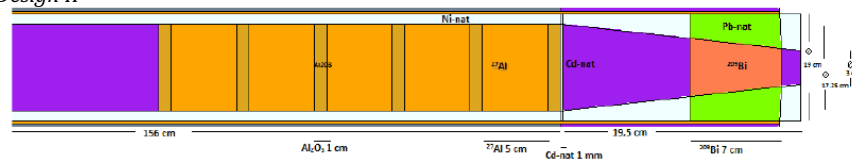**Figure 7.** Design I

4.6.2. Design II

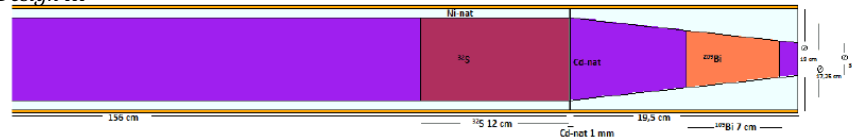**Figure 8.** Design II

4.6.3. Design III

Figure 9. Design III

This collimator design does not fully pass the IAEA's criteria, since the gamma component and fast neutron component is always below the recommended value of less than 2×10^{-13} Gy cm^2/n.

5. Conclusion

A conceptual design of moderator which is proper to be implanted in the radial piercing beam port of Kartini Research Reactor has been made. It consists of:

1. 1.75 cm thick of Ni-nat, as collimator wall
2. 5 cm thick of ^{32}S, as moderator
3. 1 mm thick of Cd-nat, as thermal and fast neutron filter

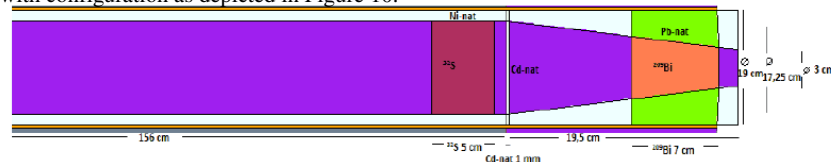4. 7 cm thick of Bi as γ-ray shielding, and with configuration as depicted in Figure 10.

Figure 10. Final Design of Moderator

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