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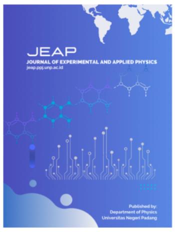

Simulation of Silicon-Rubber and Boric Acid Composite Type Neutron Shields Thermal Absorption Efficiency Using NGCal Software

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Abstract: Thermal neutron shielding is a structure or material that plays an important role in thermal neutron radiation protection to avoid the negative impact of direct radiation exposure, both on the environment and human health. In this study, radiation shielding parameters are simulated in determining the performance of fabricated neutron shielding materials using NGCal computational software. NGCal has advantages in calculation speed and ease of use, allowing efficient evaluation of parameters without requiring large computational resources. Calculations were performed by theoretical computation by varying the material ratio and thickness of the shield to be analysed to determine its efficiency. Based on the calculations performed, it can be concluded that the shield with high efficiency is the shield with the use of a higher ratio of sorbent, i.e. boric acid, while if the ratio of silicone rubber is greater than boric acid, the absorption efficiency level decreases, but the mechanical flexibility of the shield will be better. The thickness of the neutron shield is directly related to the MAC and LAC values, where the thicker the shield, the higher the MAC and LAC values, which leads to an increase in the thermal neutron absorption efficiency by the neutron shield when boric acid dominates in the composite, but when the thickness of the shield is dominated by silicone rubber, the efficiency will decrease.

Keywords: Thermal Neutron, Neutron Shiel, NGCal, Linear Damping Coefficient, Half Value Layer

1. Introduction

Neutron shielding is a structure or material that plays an important role in radiation protection by reducing particle energy and absorbing as much secondary radiation as possible [1]. Negative impacts will be caused if exposed to neutron radiation directly, both to the environment and human health, including cell damage, nerve disorders, hematopoietic syndrome, and others [2]. Neutrons are mass-neutral charged particles similar to protons [3] that are usually produced during nuclear reactions and nuclear fission. in materials neutrons interact mainly with atomic nuclei. The atomic

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structure of the material can be penetrated by neutrons without being deflected or slowed down significantly [4]. Neutron shielding causes energy deceleration until it reaches the thermal neutron energy, which is less than 0.025 eV [5]. Thermal neutrons will react with absorbing materials commonly used in thermal neutron shields, including Gd, Eu, Sm, Cd, and B. One method to produce thermal neutron shields is to combine or composite materials with neutron-absorbing isotopes [6]. Concrete, polymers, and lead are some of the basic materials that will be combined with absorbing isotopes in neutron shields to make composites [7]. To achieve high thermal neutron shielding capacity, both the absorber and the base material must meet the requirements of efficient neutron shielding.

In the manufacture of neutron shields, there are several important factors that must be considered properly because they can affect the radiation protection properties of neutron shields, namely the composition of the constituent chemicals used, the ratio of material use, shield thickness, and radiation shielding parameters [8]. Radiation shielding parameters that must be understood include mass damping factor, linear damping factor, and half-value layer [9]. Radiation shielding parameters can theoretically be determined using simulations and direct calculations from data libraries. The use of computational (simulation) software to determine the basic properties of shielding can reduce the amount of error and provide results similar to experimental results [10]. For this reason, the accuracy of information regarding the damping and protection properties of the designed neutron shield is very important to ensure the effectiveness of the shield in absorbing thermal neutrons optimally. This research is important to produce accurate and reliable data as a basis for the development of efficient neutron shields that meet the needs of practical applications.

Radiation shielding properties are conventionally calculated using macroscopic effective neutron removal cross sections, which are energy limited [11]. In addition, various computer programmes such as MERCSF-N, Phy-X, and NXcom [12], ParShield, and MRCsC have been widely used to calculate macroscopic cross sections of neutron shielding materials. These programmes rely on specific absorption cross-section data to reflect radiation protection parameters, such as damping efficiency and neutron transmission. MRCsC consisting of preprocessors and postprocessors, analytical models, and integrated databases, was developed to be an effective tool for radiation shielding design [13]. In addition, Monte Carlo-based simulations such as MCNP5, Geant4, and FLUKA [14], [15] are often used to model the interaction of particles with matter in greater detail [16]. However, these approaches require long simulation times, high technical knowledge, and sometimes commercial licences, as with MCNP5, making them less practical for simpler analysis needs. In addition, some of these programmes such as NXcom, Phy-X, and MRCsC are limited to thermal neutron energy, requiring more complex configurations for thermal neutrons.

Based on the previous problem description, we conducted a simulation study to evaluate the thermal neutron absorption efficiency of a neutron shield designed using a silicon-rubber base material and boric acid as the absorbent material. The computational software used in this study is NGCal, which simulates the properties and parameters of shielding materials for thermal neutron radiation absorption. To use NGCal effectively, accurate information is required regarding the compound's density, formula, neutron source energy, and the fraction of each compound used. NGCal offers a faster and more accessible solution for calculating shielding material parameters such as Mass Attenuation Coefficient (MAC), Linear Attenuation Coefficient (LAC), and Half-Value Layer (HVL). Unlike Monte Carlo simulations, NGCal uses a computational and mathematical approach based on radiation data libraries to provide quick, accurate calculations of material attenuation properties. This makes NGCal particularly useful for evaluating composite materials in neutron shielding applications, offering a more practical and efficient method without sacrificing accuracy. Thus, NGCal complements existing simulation tools by providing an easier-to-use, cost-effective solution for analyzing neutron shielding properties.

2. Method

The use of NGCal requires information on the chemical formula of each material used.Material preparation includes determining the most effective base and sorbent materials used in the production of thermal neutron shields, as well as preparing ten variations of material ratio and neutron shield thickness. In this study, the sorbent boric acid was combined with a silicon-rubber base material. Silicone-rubber is an elastomeric material containing the elements silicon, carbon, hydrogen, and oxygen that provides many advantages over other materials and from polymers of silicon with Si-O. Silicon is derived from liquids that are usually found in the form of polydimethylsiloxane polymers. Polydimethylsiloxane (C_2H_6OSi) is a rigid elastomeric structure with a catalyzed crosslinking reaction [17]. SR is more often used as a polymer material in radiation applications because the Si-O bonds in silicon rubber have a higher dissociation energy than C-C bonds in general [18]. The chemical structure of silicon-rubber is shown in Figure 1.

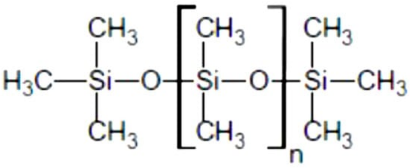


Figure 1. Silicon-Rubber Chemical Structure

Polymer composites hold significant potential for the radiation shielding industry due to their multifunctionality, adaptable shielding properties, affordability, low density, and ease of manufacture. Silicone rubber offers several advantages compared to other materials, including biocompatibility, resistance to abrasion, exceptional waterproof performance in high humidity environments, durability against weathering and oxidation, excellent resistance to extreme temperatures and chemicals, as well as strong electrical insulation properties, amon [8], [19], [20].

Boric acid is a mineral compound containing boron that occurs abundantly in nature. It primarily exists in two crystalline forms: metaboric acid (HBO_2) and orthoboric acid ($B(OH)_3$), with orthoboric acid being the more prevalent form. This compound features a layered crystal structure characterized by a combination of strong covalent, ionic, and hydrogen bonds within and between its layers [21]. The structure of boric acid is illustrated in Figure 2.

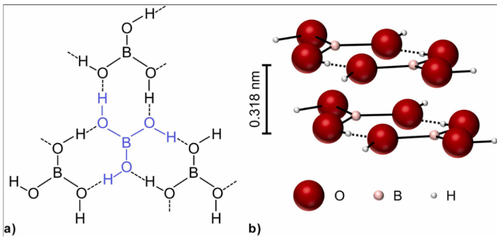


Figure 2. Boric Acid Chemical Structure

The significant thermal neutron capture cross section of the boron element in boric acid makes it efficient to use in nuclear experiments so that neutrons can be absorbed to reduce radiation risks. In addition, the properties of good chemical stability, flexibility when used in various formulations, easily soluble in water, easily available at an affordable cost, etc. are also reasons for choosing boric acid as an absorbent material in thermal neutron shields [22].

After the base material and sorbent are selected, the next step is to determine the composition of each of these materials which will be used as input data for calculations with NGCal. In this study, a material composition with 10 variations in material ratio and 10 variations in thermal neutron shield thickness was used. Boric acid powder ($B(OH)_3$) and silicon rubber (C_2H_6OSi) were used with 10 variations in the mass ratio of each material carried out at a constant thickness of 1 cm with a total volume of 1312 cm^3. The densities of boric acid and silicon rubber are 0,70 (g/ cm^3) and 0,53 (g/ cm^3), referring to calculations made by Ha et al, 2022 [23]. The composition of the required materials is shown in table 1.

Table 1. Composition of Boric Acid and Silicon Rubber at 1 cm Thickness

Mass Ratio $B(OH)_3$: C_2H_6OSi	Mass of $B(OH)_3$ (g)	Mass C_2H_6Osi (g)	Fraction of $B(OH)_3$	Fraction of C_2H_6OSi	Total Density (g/ cm^3)
1,30 : 1	460	350	0,568	0,432	0,615
1,08 : 1	414	381,9	0,520	0,480	0,607
0,88 : 1	368	416,73	0,469	0,531	0,598
0,71 : 1	322	451,55	0,416	0,584	0,590
0,57 : 1	276	486,38	0,362	0,638	0,581
0,44 : 1	230	521,2	0,306	0,694	0.573
0,33 : 1	184	556,03	0,249	0,751	0,564
0,23 : 1	138	590,85	0,189	0,811	0,556
0,15 : 1	92	625,68	0,128	0,872	0,547
0,07 : 1	46	660,5	0,065	0,935	0,538

Table 1 shows the composition of the materials that make up the thermal neutron shield at a thickness of 1 cm. It can be seen that the mass fraction of boric acid decreases from 0,568 to 0,065 and the mass fraction of silicon rubber increases along with the change in the mass ratio of materials from 0,432 to 0,935, which means that this change in composition shows a decrease in boric acid and an increase in silicon rubber in the mixture of materials. Because the density of boric acid is greater than the density of silicon rubber, from a mass ratio of 1,31 : 1 to 0,07: 1 causes a decreasing in total density. Boric acid powder ($B(OH)_3$) and silicon rubber (C_2H_6OSi) were used with 8 variations of thermal neutron shield thickness. The densities of boric acid and silicon rubber are 0,70 (g/ cm^3) and 0,53 (g/ cm referring to calculations made by Ha et al, 2022 [23]. The composition of the required materials is shown in Table 2.

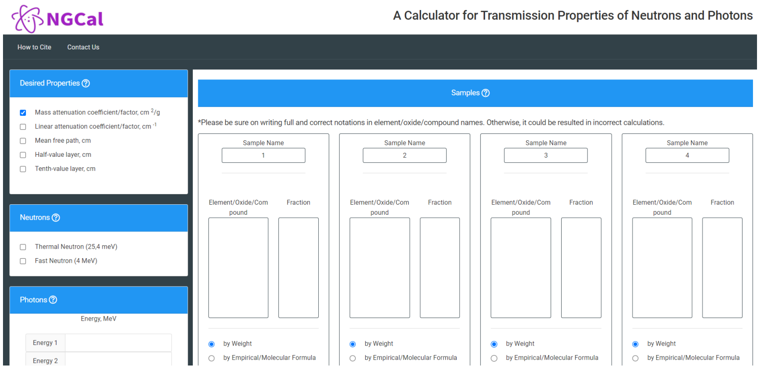
Table 2. Boric Acid and Silicone Rubber Composition at Varying Shield Thicknesses

Thickness (cm)	Mass of $B(OH)_3$ (g)	Mass of C_2H_6OSi (g)	Fraction of $B(OH)_3$	Fraction of C_2H_6OSi	Total Density (g/ cm^3)
0,2	100	30	0.77	0.23	0.652
0,4	100	75.36	0.57	0.43	0.615
0,6	100	120.72	0.45	0.55	0.596
0,8	100	166.08	0.38	0.62	0.583
1	100	211.44	0.32	0.68	0.575
1,2	100	256.8	0.28	0.72	0.569
1,4	100	302.16	0.25	0.75	0.564
1,6	100	347.52	0.22	0.78	0.560

Table 2 shows the composition of the materials that make up the thermal neutron shield. The mass of boric acid is kept constant at 100 grams, which means that the increase in shield thickness is due to the increase in silicon rubber mass. Proportionally, the mass of silicon rubber increases as the shield thickness increases. Since boric acid has a higher density value, even though the thickness of the shield increases the total density of the composite will decrease, as well as the fraction of boric acid.

2.1 Calculation Using NGCal Software

NGCal is a specialized computational tool developed to determine radiation shielding parameters, including mass and linear attenuation coefficients, mean free path, half-value layer, and tenth-value layer, for materials made of elements, compounds, and composites. It accommodates a variety of radiation sources such as X-rays, fast neutrons, thermal neutrons, and photons (encompassing both X-rays and gamma rays) [24].



☑ Mass attenuation coefficient/factor, cm ^{2}/g
☐ Linear attenuation coefficient/factor, cm $^{-1}$
☐ Mean free path, cm
☐ Half-value layer, cm
☐ Tenth-value layer, cm

☐ Thermal Neutron (25,4 meV)
☐ Fast Neutron (4 MeV)

*Please be sure on writing full and correct notations in element/oxide/compound names. Otherwise, it could be resulted in incorrect calculations.

Sample Name: 1 ● by Weight ○ by Empirical/Molecular Formula
Sample Name: 2 ● by Weight ○ by Empirical/Molecular Formula
Sample Name: 3 ● by Weight ○ by Empirical/Molecular Formula
Sample Name: 4 ● by Weight ○ by Empirical/Molecular Formula

Figure 3. NGCal Software Interface

In the NGCal software, the user is asked to input some data from the composition of the material used. The required input data includes the total density, the formula of the element, molecule or compound of the material used and the fraction of each element, molecule or compound. After that, the energy source is selected according to the experiment to be tested for neutrons and input photon values for photon radiation (X-rays and gamma rays). The output is selected according to the user's needs.

2.2 Radiation Shielding Parameters

The accuracy of information regarding the neutron attenuation properties and shielding materials of the designed thermal neutron shield is determined through an evaluation study of radiation shielding parameters, including the mass attenuation factor, linear attenuation factor, and half-value layer, all of which impact the efficiency of thermal neutron absorption by the shield. The exponential damping approach is used as the basis for estimating the mass damping coefficient. The mass attenuation coefficient (MAC) (μ / ϱ) is the probability of interaction occurring between matter and mass per unit area which is theoretically evaluated using the equation [25], [26]:

$$\mathrm{MAC} = \mu_{\mathrm{m}} = \frac{\mu}{\rho} = \frac{1}{\mathrm{x}} \ln \left(\frac{\mathrm{N_0}}{\mathrm{N}}\right) \tag{1}$$

Where $\mathrm{N_0}$ and N are the intensity before and after damping, x is the thickness of the sample. The linear attenuation coefficient (LAC) (μ_i) is the radiation intensity absorbed per unit by the thickness of the absorbing material. LAC can be obtained using the equation:

$$\mathrm{LAC} = \mu_{\mathrm{i}} = \left(\frac{\mu}{\rho}\right) \rho \tag{2}$$

MAC and LAC values are obtained from the calculation results using computational software, namely NGCal. Then calculated to get the half value layer (HVL) value with the equation:

$$\mathrm{HVL} = \frac{\ln 2}{\mu_{\mathrm{i}}} \tag{3}$$

To predict the neutron energy that can transmit a known thickness, the transmission factor (TF) is used, which is calculated by the equation:

$$\mathrm{TF} = \frac{\mathrm{N}}{\mathrm{N_0}} = \mathrm{e}^{-\mu x} \tag{4}$$

The thermal neutron radiation absorption efficiency (RPE) by the absorbing material can be calculated using the equation:

$$\mathrm{RPE} = \left|1 - \left(\frac{\mathrm{N_0}}{\mathrm{N}}\right)\right| \times 100 \tag{5}$$

3. Results and Discussion

The manufacture of thermal neutron shield composites using boric acid as an absorbent material and silicon rubber as a base material is carried out using the composition of materials in accordance with the variations made, namely variations in the ratio of materials and variations in shield thickness contained in table 1 and table 2. Based on the predetermined material composition data, theoretical calculations are performed using NGCal software to analyze the impact of varying material ratios and shield thickness on the efficiency of thermal neutron absorption by neutron shields. In addition, to determine the absorption and protection properties by neutron shields against thermal neutron radiation, an evaluation is carried out regarding several radiation shielding parameters, namely Mass Attenuation Coefficient (MAC), Linear Attenuation Coefficient (LAC), and Half Value Layer. The value of these radiation shielding parameters can be obtained using NGCal software with predetermined composition data. The calculation used a radiation source in the form of thermal neutrons with an energy of 0.025 eV.

Calculations with various material ratios were performed at a constant thickness of 1 cm, using 10 different mass variations of boric acid and silicone rubber, ranging from 1.31:1 to 0.07:1. The results obtained from the NGCal software provided MAC and LAC values, which were then used in equations 3 and 5 to determine the HVL value and thermal neutron absorption efficiency of the designed neutron shield. The calculation data can be seen in Table 3.

Table 3. Calculation of Radiation Shielding Parameters Using NGCal at 1 cm Thickness

Mass Ratio $B(OH)_3$: C_2H_6OSi	Thickness (cm)	Mass Attenuation Coefficient (MAC) (cm^2 /g)	Linear Attenuation Coefficient (LAC) (cm^{-1})	Half Value Layer (cm)	Absorption Efficiency (%)
1.31 : 1	1	7.2870428	4.481531359	0.154634643	98.868
1.08 : 1	1	7.0032214	4.250955436	0.163022175	98.575
0.88 : 1	1	6.7016612	4.007593431	0.172921733	98.182
0.71 : 1	1	6.3882751	3.769082336	0.183864383	97.693
0.57 : 1	1	6.0689760	3.526075108	0.196535802	97.058
0.44 : 1	1	5.7378511	3.287788704	0.210779969	96.266
0.33 : 1	1	5.4008132	3.046058672	0.227507108	95.245
0.23 : 1	1	5.0460365	2.805596305	0.247006313	93.953
0.15 : 1	1	4.6853468	2.562884724	0.270398428	92.292
0.07 : 1	1	4.3128312	2.320303228	0.29866786	90.176

From table 3, we can analyze that the thermal neutron absorption efficiency by the smallest neutron shield at a ratio of 0.07 : 1 with an efficiency of 90.176% and the largest absorption efficiency is at a ratio of 1.31: 1 with an absorption efficiency of 98.868%. From the data, a graph of the relationship between the mass ratio of materials with Mass Attenuation Coefficient (MAC) Linear Attenuation Coefficient (LAC), and Half Value Layer, and thermal neutron absorption efficiency was obtained.

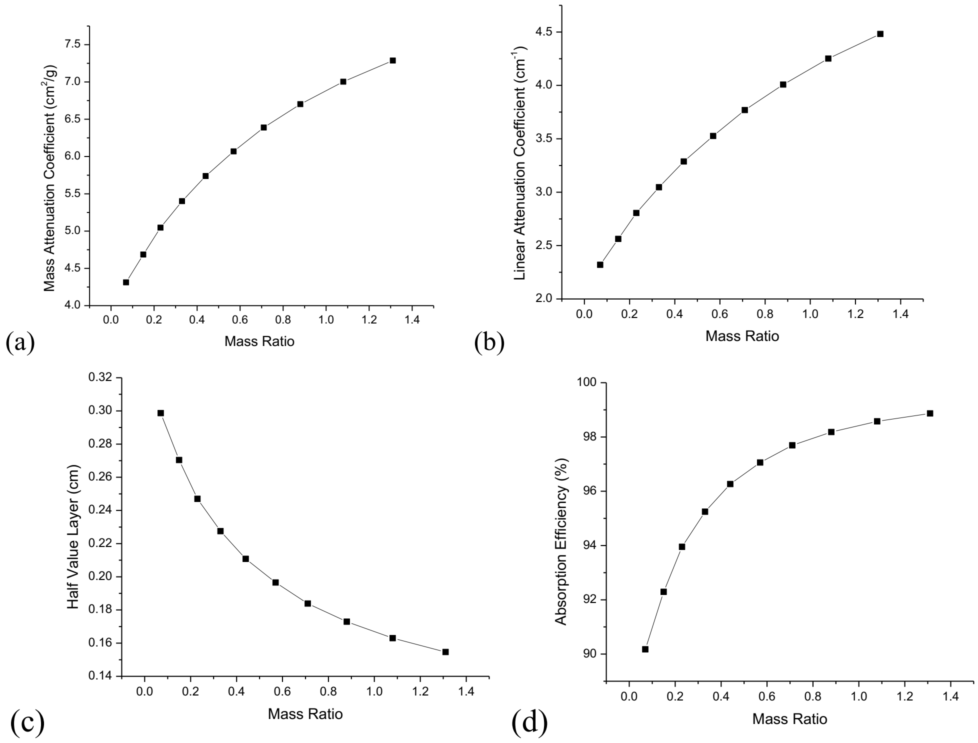


Figure 4. Relationship Graph between Mass Ratio and (a) Mass Attenuation Coefficient (b) Linear Attenuation Coefficient (c) Half Value Layer (d) Absorption Efficiency

From Figures 4 and 5, it can be analyzed that a decrease in the mass ratio of boric acid to silicon rubber causes a decrease in the MAC and LAC values of the designed shield. The Linear Attenuation Coefficient (LAC) value is directly linked to the shield's absorption efficiency, a lower LAC value indicates a decrease in the efficiency of thermal neutron absorption by the shield. As for the HVL on decreasing the material mass ratio, the HVL value obtained is increasing which means that the absorption efficiency of the neutron shield will decrease along with the increase in the HVL value obtained because the increase in HVL indicates that the material requires a greater thickness to achieve the same absorption rate. The ratio of the mass ratio of boric acid to silicon rubber can be used according to the application. In theory boric acid acts as an effective filter material for use in thermal neutron radiation shields, which means that composites with a greater ratio of boric acid will be more effectively used in thermal neutron shields. Meanwhile, if the mass ratio of silicon rubber is more than boric acid, it causes a reduction in the efficiency of the shield made, but makes the shield have a high level of flexibility.

Calculations with variations in shield thickness were carried out with a variation of 10 data, namely at a thickness of 0.2 cm to 2 cm. The calculation results in NGCal software produce MAC and LAC values that can be calculated into equations 3 and 5 to obtain the HVL value and thermal neutron absorption efficiency by the designed neutron shield.The calculation data can be seen in Table 4.

Table 4. Calculation of Radiation Shielding Parameters Using NGCal with Variations in Shield Thickness

Thickness (cm)	Mass Attenuation Coefficient (MAC) (cm^2 /g)	Linear Attenuation Coefficient (LAC) (cm^{-1})	Half Value Layer (cm)	Absorption Efficiency (%)
0.2	8.48145785	5.52991052	0.125	99.603
0.4	7.29886875	4.48880428	0.154	98.877
0.6	6.58931529	3.92723191	0.176	98.030
0.8	6.17540911	3.60026351	0.192	97.268
1	5.82063238	3.34686362	0.207	96.481
1.2	5.58411456	3.17736118	0.218	95.830
1.4	5.40672619	3.04939357	0.227	95.261
1.6	5.22933783	2.92842918	0.237	94.652

From Table 4, we can analyze that the absorption efficiency of thermal neutrons by the neutron shield decreases as the shield thickness increases. This shows that although increasing the shield thickness can increase the overall neutron absorption, there is a decrease in efficiency at higher thicknesses. From the data, a graph of the relationship between shield thickness and Mass Attenuation Coefficient (MAC) Linear Attenuation Coefficient (LAC), and Half Value Layer, as well as thermal neutron absorption efficiency was obtained.

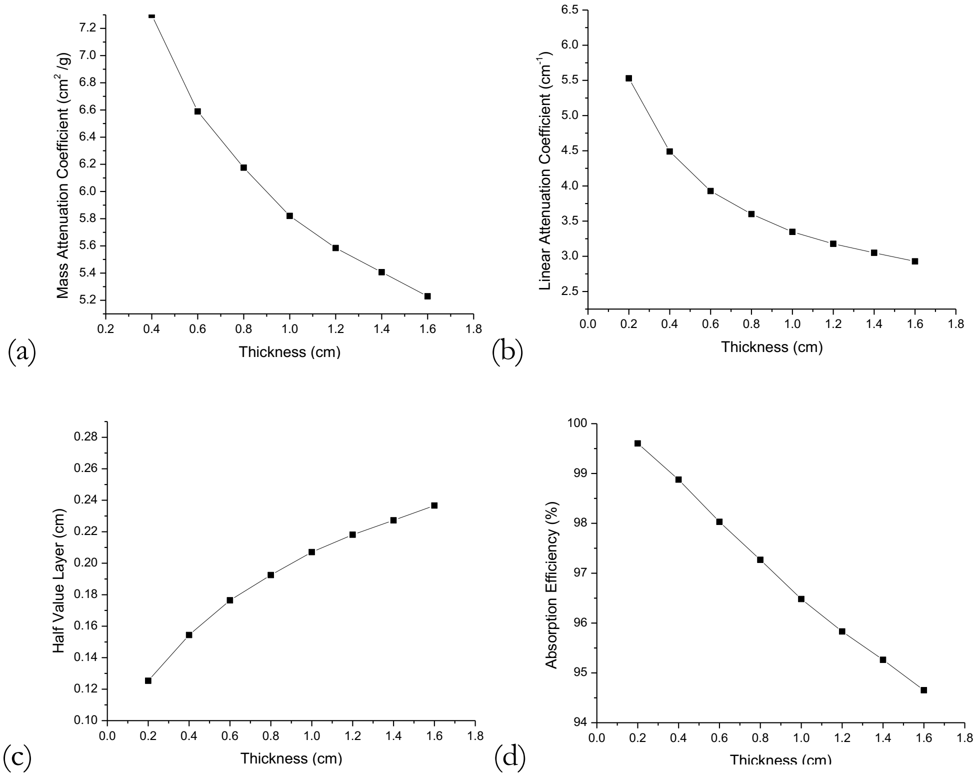


Figure 5. Graph of Relationship Between Thickness and (a) Mass Attenuation Coefficient (b)Linear Attenuation Coefficient (c)Half Value Layer (d)Absorption Efficiency

From Figure 5, it is known that the relationship between shield thickness and MAC and LAC values is inversely proportional, where MAC is the effectiveness of the material in absorbing radiation per unit mass and LAC is the effectiveness of the material in absorbing neutron radiation per unit length. Because in the designed neutron shield composite, the mass of boric acid as the absorbing material is made constant, along with the increase in shield thickness, the material that dominates at a greater thickness is silicon rubber which does not have the ability to absorb thermal neutrons [18] so that the increase in thickness causes a decrease in MAC and LAC values.

The decrease in LAC and MAC values is in line with the absorption efficiency by the neutron shield, where in this design, the thickness of the neutron shield is inversely proportional to its absorption efficiency. This can be attributed to several factors. The addition of silicone rubber with increasing thickness reduces the concentration of boric acid in the composite, leading to a decrease in absorption efficiency. Silicone rubber contributes to the shield as a whole by increasing the thickness of the material. However, as its proportion increases, less boric acid is available to absorb neutrons, resulting in a decrease in thermal neutron absorption efficiency.

The relationship between thickness and HVL (Half-Value Layer) is directly proportional. HVL is defined as the thickness required to reduce the radiation intensity to half of its initial value [27]. With a decrease in LAC, a greater thickness is required to achieve the same reduction in radiation intensity. Therefore, as the proportion of silicone rubber increases along with the shielding thickness, the HVL also increases, which confirms that a thicker material is needed to effectively dampen radiation. Smaller HVL values correspond to higher thermal neutron absorption efficiency, which emphasizes the importance of optimizing the material composition and thickness of the shield.

From a design perspective, increasing shield thickness does improve radiation protection in general, but there are practical limitations such as additional base material, weight of the resulting shield and material cost. Thus, the optimal approach is to determine the minimum thickness that can still provide the desired absorption efficiency, based on protection parameters such as HVL. The combination of theoretical approaches with simulation, as done with NGCal, allows researchers to rapidly dial in a wide variety of thicknesses and material compositions without the need to conduct time-consuming and costly physical experiments. In addition, adjustments to material ratios can provide challenges in meeting application-specific needs. For example, increasing the amount of boric acid can increase the MAC and LAC at a certain thickness, but this can also eliminate the mechanical properties of the shield, such as elasticity or resistance to cooling. Using software such as NGCal, compositional variations can be described in detail to achieve a balance between shielding properties and mechanical properties, resulting in an efficient and applicable neutron shielding solution.

Validation of the calculation parameters using NGCal is done by considering the data to be used in the calculation such as material composition, density, and neutron source energy, which are then entered into the software. NGCal will use the relevant material absorption cross-section data to calculate parameters such as Mass Attenuation Coefficcient (MAC), Linear Attenuation Coefficcient (LAC), and Half-Value Layer (HVL) based on predefined calculations. The results of these calculations can then be tested by comparing them with the calculation data using the corresponding equations from the previously described references. Thus, validation is performed by ensuring that the results obtained from NGCal are consistent and in line with the results of calculations that have been widely accepted in the scientific literature.

4. Conclusion

The manufacture of high-efficiency thermal neutron shields requires accurate calculation of the absorption and protection properties of the designed shield. The factors that affect the absorption efficiency of thermal neutrons are the selection of absorbent materials with high absorption cross-sections and good base materials. In addition, the thickness of the shield and the mass ratio of the materials used also directly affect the value of the radiation shielding parameters to be evaluated, namely Mass Attenuation Coefficient (MAC), Linear Attenuation Coefficient (LAC), and half value layer which will affect the thermal neutron absorption efficiency by the shield. By using NGCal software, the required values of radiation shielding parameters can be accurately obtained. Based on the calculations carried out, it can be concluded that shields with high efficiency are shields with the use of a higher ratio of absorbent material, namely boric acid, while if the ratio of silicone rubber is greater than boric acid, the absorption efficiency level decreases, but the mechanical flexibility of the shield will be better. The thickness of the neutron shield is directly related to the MAC and LAC values; as the shield becomes thicker, both MAC and LAC values increase, leading to improved thermal neutron absorption efficiency when boric acid dominates the composite. However, if silicon rubber predominates, increasing the thickness may actually reduce the absorption efficiency.

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