

Design and Performance Study of Carbon-Containing Neutron Shielding Materials

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Abstract

In this paper, Monte Carlo method is used to simulate the shielding effect of various shielding materials on high energy neutron by using MCNP5. In the experiment, it is found that the density of composite material is very difficult to improve, the shielding effect of material is far inferior to that of layered design, so the design of this paper is layered. The optimum thickness of different materials is obtained by counting the energy and selecting different shielding materials for different energies. The main research contents are as follows: Firstly, the shielding effect of iron, aluminum, graphite and polyethylene on neutron with different energy is studied, and the results show that the shielding effect of heavy nuclei is better for high energy neutron. Compared to aluminum and iron, found that the use of iron is better, and when the thickness of 24 cm, 14 MeV Neutron shielding after the remaining less than five out of 10,000. Therefore, the first layer of material selection of iron, thickness of 24 cm. It is found that the shielding effect of light nuclei is good for medium neutron. For the neutron around 2 MeV, the shielding effect of polyethylene is better than that of iron. When only 24 cm iron, the maximum count is 0.5 MeV, after shielding neutron count is 0.06; When adding 8 cm polyethylene, the maximum count in 0.5 MeV, after shielding counting only 0.001, but still exist in the lower energy segment peak, thermal neutron count of 0.02, so the need. When the boron carbide thickness is 3 cm, the 0.5 MeV neutron count and the thermal neutron count are already very low. When the outermost iron is 12 cm, the maximum count of 0.5 MeV neutron count has dropped to 2000 points. In short, the results of the design of 14 MeV high energy neutron are as follows, such as Iron 24 cm, polyethylene 8 cm, boron carbide 3 cm, iron 12 cm, the effect of layered composite shielding is ideal.

Keywords

Neutron Shielding; Transmission Coefficient; Carbon Containing Materials; MCNP5.

1. Introduction

With the continuous advancement of nuclear physics research, the applications of nuclear energy and nuclear technology have become increasingly widespread in fields such as medicine, aerospace, and agriculture. Neutrons, as high-energy particles produced in nuclear reactions, exhibit significant advantages due to their unique physical properties: (1) Neutrons possess strong penetration capabilities, enabling non-destructive testing of thick metallic materials; (2) Characteristic γ -rays generated through absorption or inelastic collisions can distinguish between isotopes and elements with similar atomic numbers; and (3) Fast neutrons are sensitive to light elements, and their interaction with resonance absorption of light elements produces γ -rays, allowing for the detection of the distribution and concentration of light elements in materials. Leveraging these properties, neutron technology has found extensive applications in neutron scattering spectrometers, neutron CT, neutron activation, and other areas [1].

However, the high energy and strong penetration of neutrons also pose significant challenges for radiation shielding. Neutron shielding is typically divided into two stages: In the first stage, high-energy neutrons undergo inelastic scattering with moderating materials, losing energy and further slowing down through elastic scattering with hydrogen-rich substances. In the second stage, neutron-absorbing materials are employed to achieve the final absorption of neutrons. Since the absorption of thermal neutrons generates γ -rays, ideal absorbing materials should exhibit a high thermal neutron absorption cross-section and low capture γ -ray energy [2]. Consequently, research on neutron shielding materials has garnered considerable attention. These materials are not only applied in the construction of reactor buildings and equipment protection but also in the development of protective clothing for personnel operating neutron-related devices, ensuring the safe utilization of neutron technology.[3,4]

Conventional neutron shielding materials primarily consist of simple compounds composed of low atomic number elements, including water, polyethylene, boron carbide, and boric acid, as well as metallic materials such as stainless steel, iron, lead, and cement-based composites.[5] Compounds comprising low-Z elements demonstrate superior fast neutron moderation capabilities and effective thermal neutron absorption properties. Furthermore, boron-enriched polymeric materials exhibit not only enhanced shielding efficacy against both fast and thermal neutrons but also demonstrate favorable processability and stable physical characteristics.[6] Regarding substrate selection, cement-based materials have been extensively utilized due to their cost-effectiveness, local availability, high compositional tunability, and satisfactory structural-shielding synergy. Contemporary shielding systems predominantly employ modified cement composites incorporating functional additives, exemplified by boron-doped cement and polyethylene-reinforced cement formulations.[7]

In addition to material selection, the architectural configuration of shielding systems, whether employing monolithic materials or multilayered composites, requires systematic evaluation. Monolithic shielding structures often incur excessive mass and volumetric footprint due to the inherent limitations of single-material performance optimization. Conversely, stratified composite systems demonstrate enhanced engineering efficiency.[8,9] The primary layer reduces neutron energies below 1 MeV through inelastic scattering, subsequent layers facilitate thermalization of epithermal neutrons via moderated elastic collisions, terminal layers incorporate gamma-attenuating components to absorb secondary gamma radiation generated during neutron capture processes. Stratified composite systems achieves optimal performance-to-mass ratios, layer-specific functionalization enables targeted utilization of material properties. [10-12]

2. Selection and Design of Shielding Materials for High-Energy Neutrons

With the rapid global development of nuclear technology, significant progress has been made in neutron-related research, particularly in fields such as radiological medicine and neutron flaw detection. Concurrently, 14 MeV neutrons generated by accelerator reactions have been extensively utilized. This study focuses on investigating the shielding of 14 MeV neutrons. The shielding performance of materials can be evaluated by comparing the transmission coefficients of neutrons passing through them. [13] However, due to limitations in laboratory conditions and potential experimental errors, this study employs the MCNP5 software to simulate the shielding effectiveness of various materials and composite shielding configurations against neutrons, thereby substituting for physical laboratory experiments.[14] For this simulation experiment, materials such as polyethylene, aluminum, iron, and graphite were selected. The densities of the chosen materials are as follows: polyethylene has a density of 0.93 g/cm^3 , aluminum has a density of 2.702 g/cm^3 , iron has a density of 7.87 g/cm^3 , and graphite has a density of 2.25 g/cm^3 . When neutrons pass through a material or shielding

medium, a portion of the neutrons are absorbed, while the remaining neutrons penetrate the material. The ratio of the number of neutrons that penetrate the material to the total number of incident neutrons is defined as the neutron transmission coefficient.[15]

In MCNP5, the shielding performance of the analyzed materials against 14 MeV neutrons was simulated.

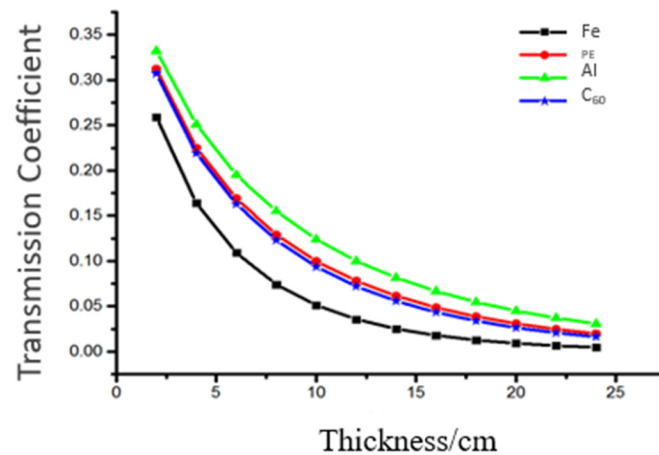


Fig 1. Variation of Transmission Rate of 14 MeV Neutrons with Thickness for Different Materials

Figure 1 shows the variation curves of the transmission rate of 14 MeV neutrons with material thickness for the four materials. As depicted in Figure 1, the transmission coefficient of each material decreases with increasing thickness. However, at all thicknesses, iron exhibits the best shielding performance, followed by graphite, polyethylene slightly inferior to graphite, and aluminum showing the poorest shielding effect. Although there are differences in the shielding performance between polyethylene and graphite, the overall disparity is minimal. Beyond 20 cm, the transmission coefficients of all four materials tend to stabilize. When fast neutrons interact with matter, reactions such as elastic scattering and inelastic scattering can occur. Among the selected materials, iron demonstrates the most effective shielding against 14 MeV neutrons.

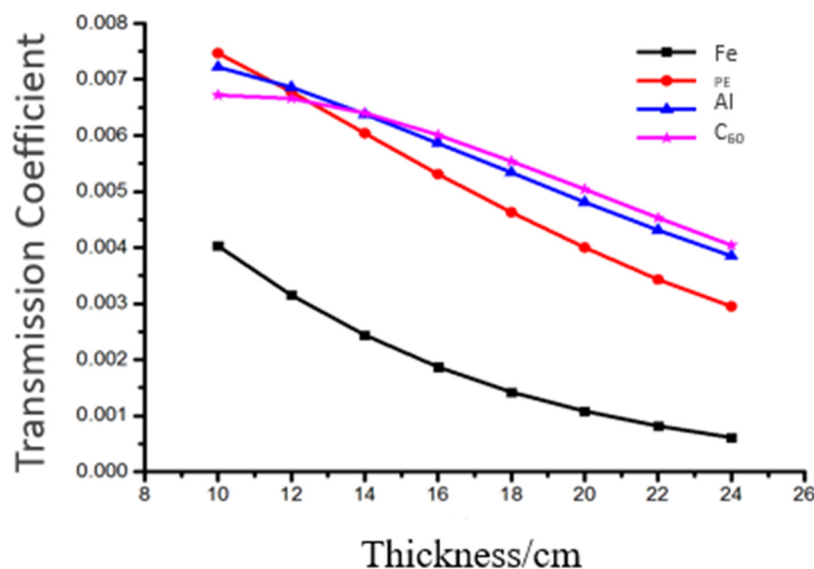


Fig 2. Variation of Transmission Rate of 5 MeV Neutrons with Thickness for Different Materials

Figure 2 presents the variation curves of the transmission coefficient for 14 MeV neutrons with thickness for the four materials. As shown in Figure 2, for thicknesses below 12 cm, the shielding effectiveness from best to worst is iron, graphite, aluminum, and polyethylene. Between 12 cm and 14 cm, the order changes to iron, polyethylene, graphite, and aluminum. Beyond 14 cm, the shielding effectiveness ranks as iron, polyethylene, aluminum, and graphite. As the thickness increases, the energy of the remaining neutrons decreases to a certain level, leading to an increase in the neutron absorption cross-section with hydrogen. Consequently, beyond 14 cm, polyethylene exhibits better shielding performance than graphite and aluminum. Clearly, for 5 MeV neutrons, iron remains the most effective shielding material. However, as the thickness increases and the energy of a portion of the neutrons decreases, the shielding effectiveness of polyethylene gradually approaches that of iron.

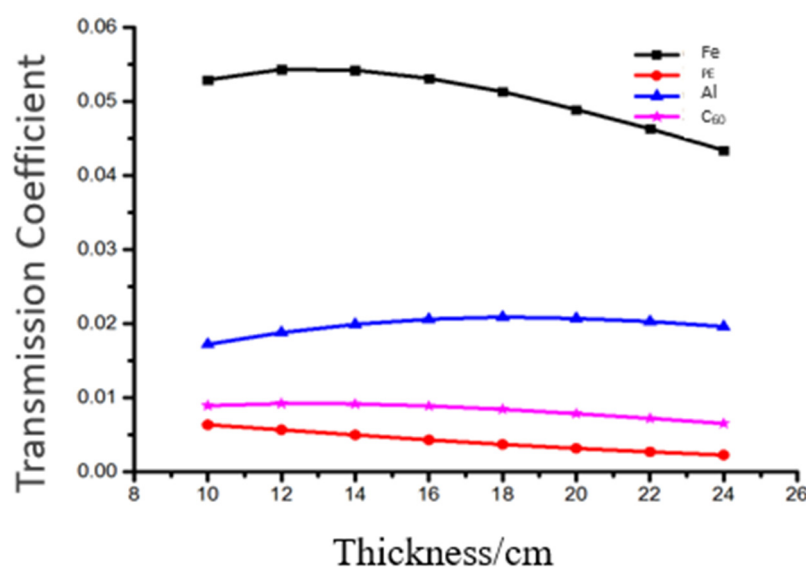


Fig 3. Variation of Transmission Rate of 1 MeV Neutrons with Thickness for Different Materials

Figure 3 illustrates the variation curves of the transmission coefficient for 1 MeV neutrons with thickness for the four materials. As shown in Figure 3, the shielding effectiveness of the four materials, ranked from best to worst, is polyethylene, graphite, aluminum, and iron. In the previous simulation, iron demonstrated superior shielding performance for 14 MeV neutrons; however, for 1 MeV neutrons, its shielding effectiveness is significantly inferior to the other three materials. When the neutron energy is low, the absorption cross-section and elastic scattering cross-section between hydrogen and neutrons dominate. Consequently, polyethylene exhibits better shielding performance than the other materials under these conditions.

From the shielding results of these materials at different neutron energies, it can be concluded that for high-energy neutrons, heavy nuclei such as iron exhibit superior shielding performance, while for low-energy neutrons, light nuclei provide better shielding effectiveness. This observation aligns with the theoretical principles of neutron shielding. In the next step, we will combine the advantages of light and heavy nuclei to investigate the shielding effectiveness of composite materials against 14 MeV neutrons and compare it with that of single materials.

For stratified composite systems, the first layer is composed of either iron or aluminum, and the MCNP5 simulation is used to compare the performance of these two materials and determine the optimal thickness for the selected material. The second layer is chosen to be either polyethylene or boron carbide-doped polyethylene, with their performance compared

and appropriate thicknesses determined. Additionally, since this study focuses on the shielding effectiveness of carbon-containing materials, a comparison between boron carbide-doped polyethylene and borax-doped polyethylene is also conducted. The densities of the selected materials are as follows: borax has a density of 2.7 g/cm^3 , and boron carbide has a density of 2.52 g/cm^3 .

2.1. Moderation of High-Energy Neutrons

For the moderation of high-energy neutrons, materials composed of heavy nuclei are required. This section primarily focuses on comparing aluminum and iron to determine the appropriate material thickness and identify the most suitable material

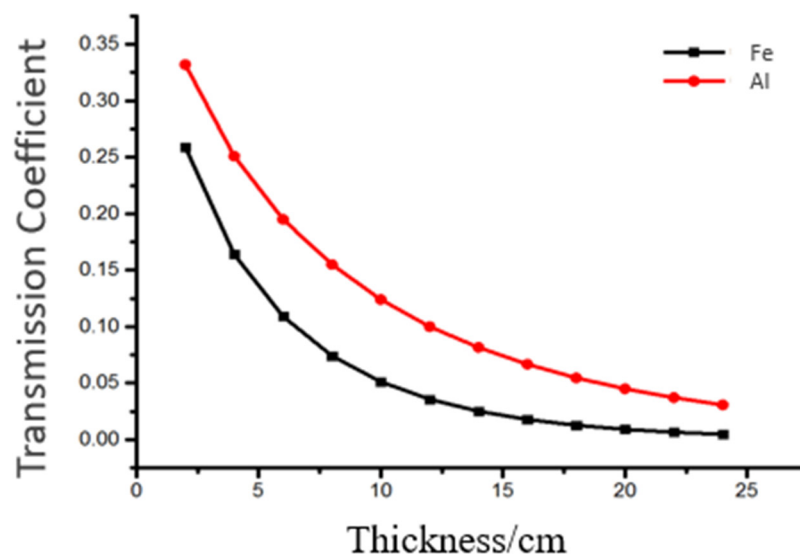


Fig 4. Comparison of Transmission Coefficient Variation with Thickness for Iron and Aluminum at 14 MeV

Figure 4 shows the variation curve of the transmission coefficient with iron thickness for 14 MeV neutrons. As illustrated in Figure 4, the transmission rate decreases rapidly with increasing iron thickness below 10 cm, indicating a significant improvement in shielding effectiveness. The transmission coefficient drops from 0.259091 to 0.051154. Between 10 cm and 20 cm, the rate of decrease slows but remains noticeable, with the transmission coefficient decreasing from 0.259091 to 0.00902187, a reduction of 96.52%. However, beyond 20 cm, the decrease becomes less pronounced. At 24 cm, the transmission rate is only 0.00182595 lower than at 22 cm, suggesting that further increases in thickness provide negligible improvements in shielding performance. For the 14 MeV neutrons studied in this work, the simulation results indicate that when the iron thickness reaches 24 cm, the transmission coefficient is reduced to 0.462733%.

Figure 4 illustrates the transmission coefficient curve of aluminum thickness when the neutron energy is 14 MeV. As shown in Figure 4, the transmission coefficient decreases gradually with increasing thickness and eventually stabilizes. Before 14 cm, the transmission coefficient shows a significant downward trend, indicating that thickness has a substantial impact on the shielding effect. The transmission coefficient drops from 0.332 to 0.0816 within this range. Between 14 cm and 30 cm, the decrease in the transmission coefficient becomes less pronounced, with the value falling from 0.0816 to 0.017. However, a visible downward trend is still observed in the figure, which continues until 36 cm, where the transmission coefficient only decreases by 0.002 compared to 34 cm. When aluminum is used as a shielding material, the transmission coefficient remains essentially unchanged

when the thickness exceeds 36 cm. At this point, the neutron energy is below 1 MeV, and the primary interaction with the material is elastic scattering. Adding other light-nuclear materials instead of further increasing the thickness of aluminum would be more effective. When the aluminum thickness is 24 cm, the transmission coefficient is 3.07%. Even when the aluminum thickness reaches 36 cm, the transmission coefficient is 1.01203%, which is still higher than that of iron.

Based on the previous simulations of iron and aluminum for neutron shielding, it has been determined that when shielding neutrons with an energy of 14 MeV, a thickness of 24 cm is appropriate for the first layer of iron shielding, while a thickness of 36 cm is suitable for the first layer of aluminum shielding. However, these two simulations did not provide a direct comparison of the shielding effectiveness of these two materials. Therefore, in the next step, we will conduct a comparative analysis of these two materials to identify the better candidate for the first layer of shielding.

In this section, simulations were conducted to compare iron and aluminum, providing a more intuitive analysis of the shielding effectiveness of these two metallic materials against neutrons with an energy of 14 MeV. The optimal shielding thicknesses were calculated for each material. By combining the simulated transmission coefficients with considerations of economic feasibility, the appropriate thicknesses of the materials were selected.

Figure 4 presents the variation of transmission coefficients with thickness for iron and aluminum when the neutron energy is 14 MeV. As shown in Figure 4, for the shielding of 14 MeV neutrons, the transmission coefficient curve for iron decreases rapidly below 8 cm. Between 8 cm and 20 cm, the rate of decrease becomes slower, but a clear downward trend with increasing thickness is still evident in the figure. The curve for iron begins to level off at 24 cm. Similarly, for aluminum, the transmission coefficient decreases significantly before 14 cm and then levels off. Overall, the transmission coefficient of iron remains lower than that of aluminum with increasing thickness, especially between 4 cm and 14 cm, where the transmission coefficient of iron is significantly lower than that of aluminum. Therefore, iron was chosen as the material for the first layer of shielding.

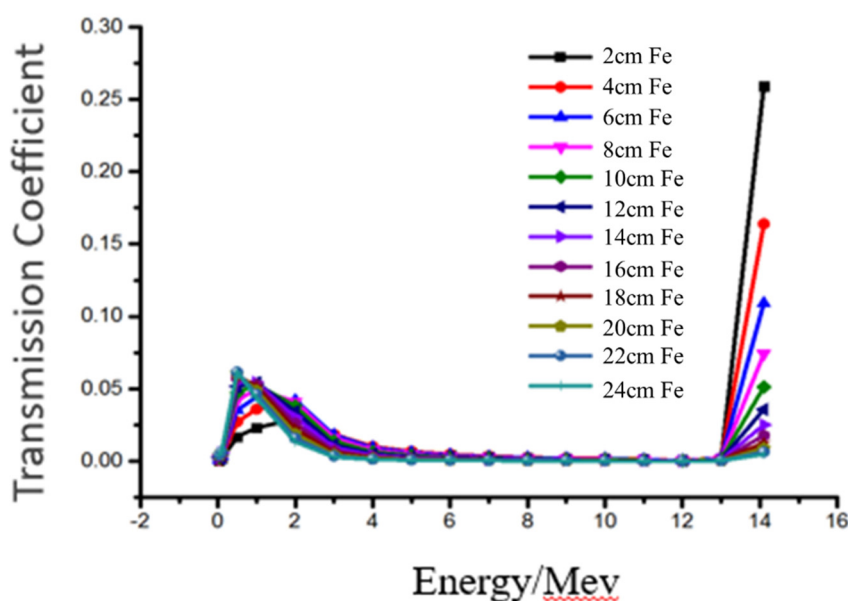


Fig 5. Transmission Coefficient Variation with Neutron Energy for Different Thicknesses of Iron

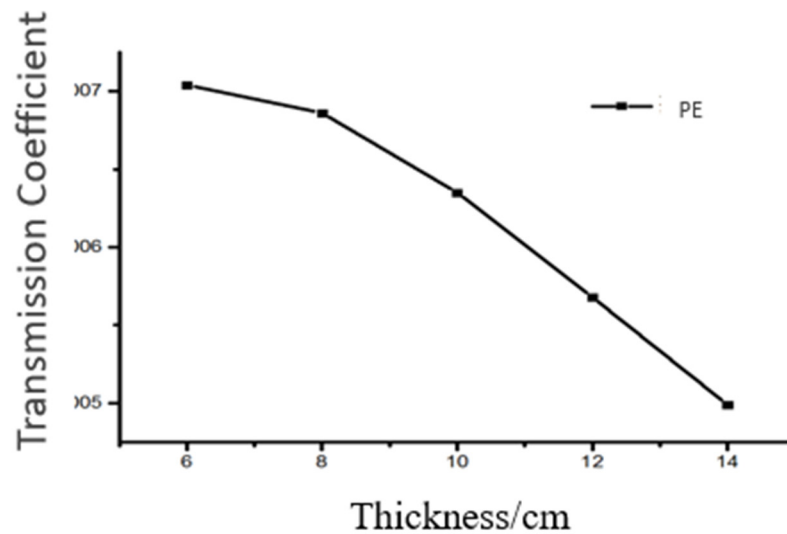


Fig 6. The curve of transmission coefficient variation with thickness of polyethylene at 1 MeV neutron energy

Figure 5 shows the variation of transmission coefficients with neutron energy for iron at different thicknesses. As indicated in the figure, although iron demonstrates effective shielding for high-energy neutrons, its performance is less satisfactory for neutrons with energies around 2 MeV. Based on the findings from the previous section, polyethylene exhibits superior shielding effectiveness for neutrons within this energy range. A comparison of Figures 5 and 6 reveals that polyethylene effectively complements iron by providing better shielding for the energy range where iron's performance is weaker. Therefore, polyethylene is selected as the material for the second layer of shielding.

2.2. Attenuation of Intermediate-Energy Neutrons

After the first layer of shielding material (iron) attenuates 14 MeV neutrons, the shielding effectiveness for neutrons around 2 MeV is not satisfactory. Based on the calculations in the previous step, polyethylene was determined as the material for the second layer of shielding. In this step, simulations were conducted to determine the optimal thickness of polyethylene when used in a dual-layer shielding configuration.

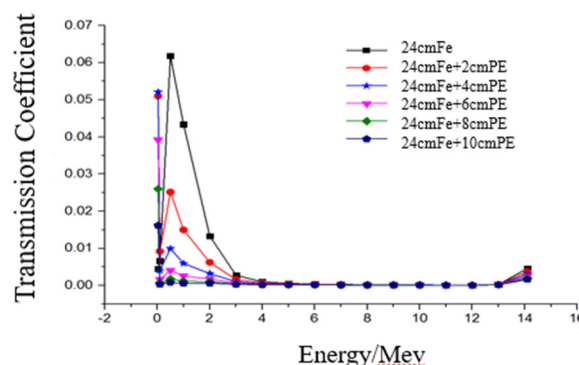


Fig 7. The energy distribution diagram of iron coated with polyethylene of various thicknesses

As shown in Figure 7, for neutrons around 2 MeV, the transmission coefficient decreases gradually with increasing thickness of polyethylene. A clear distinction in shielding performance can be observed between configurations with and without polyethylene, indicating that the addition of polyethylene significantly enhances the overall shielding

effectiveness. Although the transmission coefficient continues to decrease with increasing thickness, the reduction in transmission between 8 cm and 10 cm of polyethylene is minimal. Therefore, a thickness of 8 cm of polyethylene is deemed sufficient for effective shielding.

Specifically, when the thickness of polyethylene is 8 cm, the transmission coefficients for neutrons with energies of 0.5 MeV, 1 MeV, and 2 MeV are 0.00180001, 0.00121905, and 0.00103643, respectively. These values indicate a highly satisfactory shielding performance. Consequently, considering both shielding effectiveness and material efficiency, an 8-cm thickness of polyethylene is determined to be the optimal choice for the second layer of shielding.

2.3. Thermal Neutron Absorption

After passing through the first two layers of shielding, although polyethylene demonstrates effective moderation of neutrons around 2 MeV, its shielding performance for thermal neutrons is not satisfactory. Boron carbide (B_4C) has a large absorption cross-section for thermal neutrons and emits low-energy gamma rays upon absorption. Therefore, incorporating B_4C or borax into the third layer can significantly enhance the overall shielding effectiveness. In the subsequent simulation calculations, iron was chosen as the material for the fourth layer (outermost layer) for two main reasons: first, to shield against secondary photons generated during the shielding process; and second, because the materials used in the middle two layers are powdery and require a metallic shell to encapsulate them. Thus, iron serves both as a shielding material and a structural framework for the composite shielding system.

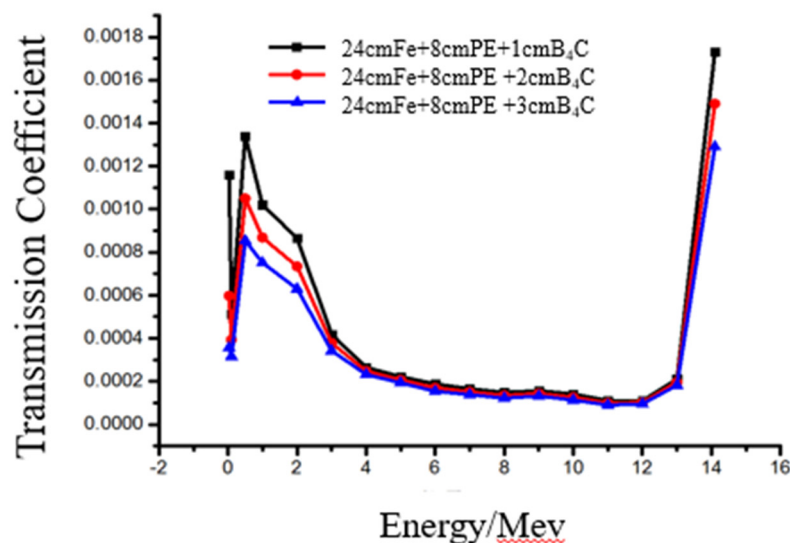


Fig 8. Transmission Coefficient Variation with Energy for Different Boron Carbide Additions

As indicated by the trend in Figure 8, within the energy range of 0–2 MeV, the transmission coefficient decreases significantly with increasing thickness of boron carbide (B_4C), especially for neutrons with energies below 1 MeV. For instance, when the neutron energy is 0.1 MeV, the transmission coefficient drops to 0.000315813 with a 3-cm thickness of B_4C , approaching one ten-thousandth. This level of shielding effectiveness is considered ideal, and further thickness increase is unnecessary.

2.4. Comparison of Shielding Effectiveness with Each Additional Layer

Figure 9 shows the curves of transmission coefficient variation with energy after each layer of shielding material is added.

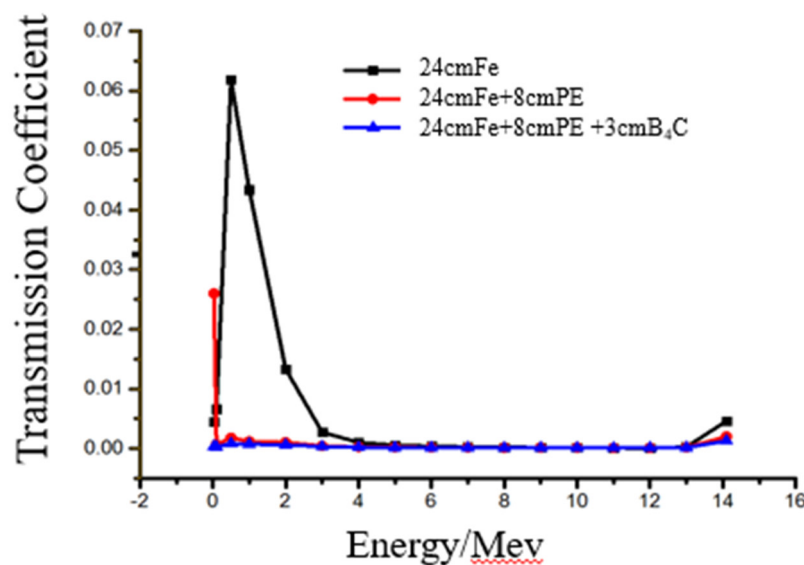


Fig 9. Figure showing the variation of transmission coefficient with energy for each added layer of shielding material.

As shown in Figure 9, when the shielding material consists only of a single layer of 24 cm of iron, the shielding effectiveness is relatively poor for neutrons around 2 MeV but is satisfactory for neutrons with energies above 4 MeV. Simulations indicate that for neutrons with an energy of 0.5 MeV, the transmission coefficient is 0.0618134, while for neutrons with an energy of 13 MeV, the transmission coefficient is 0.000298378. However, when an additional layer of 8 cm of polyethylene is added as the second layer, the shielding effectiveness for neutrons around 2 MeV is significantly improved compared to the single layer of 24 cm of iron. Specifically, the transmission coefficient for 0.5 MeV neutrons decreases to 0.00180001, representing a reduction of 97.1% compared to the single layer of iron. Despite this improvement, the shielding performance for neutrons with energies below 1 MeV remains inadequate, as evidenced by a transmission coefficient of 0.025998 for neutrons with an energy of 0.03 MeV. When a third layer of 3 cm of boron carbide is added, Figure 9 shows a marked enhancement in shielding effectiveness for neutrons with energies below 1 MeV, with the transmission coefficient approaching zero. Simulations reveal that for neutrons with an energy of 0.03 MeV, the transmission coefficient is 0.000357094, which is a 98.6% reduction compared to the configuration with 24 cm of iron and 8 cm of polyethylene. Overall, Figure 9 demonstrates that the combination of 24 cm of iron, 8 cm of polyethylene, and 3 cm of boron carbide provides excellent shielding performance for both low- and high-energy neutrons, with transmission coefficients consistently around 0.0001.

2.5. Shielding of Gamma Rays

According to the simulation process in MCNP, it is evident that gamma rays are produced during the interaction of neutrons with materials. Therefore, in addition to the shielding of neutrons with different energies as discussed previously, the shielding of gamma rays must also be considered. This layer of material not only serves to shield gamma rays but also acts as a supporting structure. Similar to the first layer, iron is chosen for this layer due to its effective gamma-ray attenuation and structural integrity.

As shown in Figure 10, the peak count rate occurs at an energy of 0.5 MeV for all thicknesses. According to Figure 11, the transmission coefficient decreases significantly with increasing thickness below 6 cm. However, between 6 cm and 12 cm, the rate of decrease gradually diminishes. When the thickness reaches 11 cm, the transmission coefficient is 0.000845857. At 12 cm, the transmission coefficient further reduces to 0.000673319, with only a marginal

difference of 0.00017. Given that the shielding effectiveness improves only slightly with additional thickness beyond 12 cm, and considering that the transmission coefficient is already sufficiently low at 12 cm, a thickness of 12 cm is deemed appropriate for the fourth layer. Therefore, the material selected for the fourth layer is 12 cm of iron.

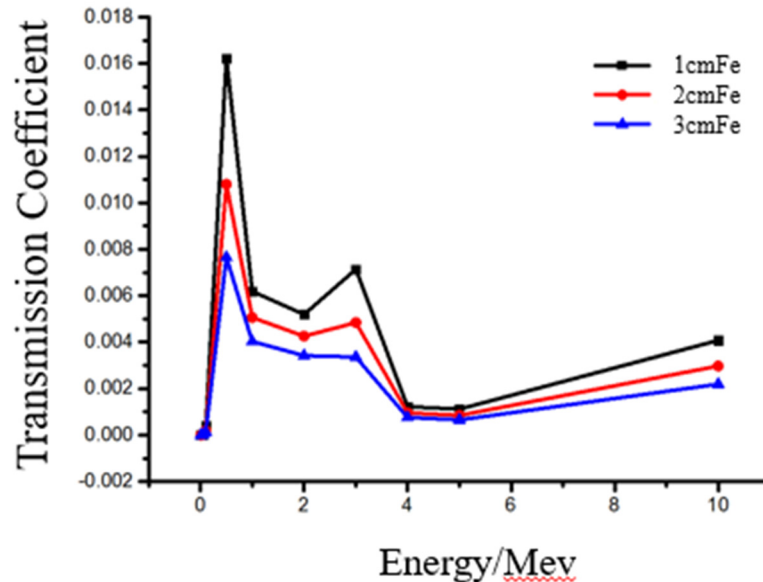


Fig 10. Variation of Transmission Coefficient with Energy for Different Thicknesses of Iron

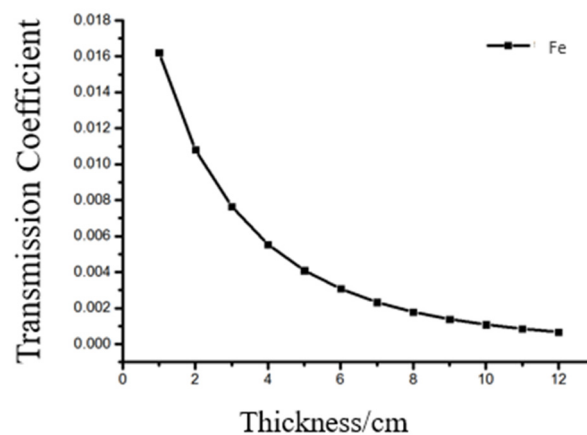


Fig 11. Transmission Coefficient Variation with Thickness at an Energy of 0.5 MeV

3. Conclusion

In this study, the Monte Carlo-based MCNP5 code was employed to simulate the shielding performance of iron, boron carbide, polyethylene, and graphite. Based on the simulation results and comparative analyses, a multi-layered neutron shielding model was designed. The main conclusions are as follows:

1. **Material Selection Based on Neutron Energy:** Comparisons of shielding effectiveness among different materials across various neutron energies revealed that heavy nuclei (nuclei with large mass numbers) are more effective for high-energy neutrons, while light nuclei (nuclei with small mass numbers) perform better for low-energy neutrons. Therefore, iron was selected as the first layer, polyethylene as the second layer, and boron carbide as the third layer.
2. **Optimal Thickness for First Layer:** Using MCNP5 simulations, the appropriate thicknesses for iron and aluminum as the first layer shielding material against 14 MeV

neutrons were determined to be 24 cm and 36 cm, respectively. Despite the thicker aluminum layer, the transmission coefficient for iron was 0.00462733, compared to 0.0101203 for aluminum. This indicates that iron provides better shielding effectiveness. Thus, iron was chosen as the first layer material with a thickness of 24 cm.

3. **Enhanced Shielding with Polyethylene:** It was found that polyethylene outperforms iron in shielding neutrons around 2 MeV. For instance, with only 24 cm of iron, the maximum neutron count rate was 0.0618134 at 0.5 MeV. When an additional 8 cm of polyethylene was added, the count rate at 0.5 MeV decreased to 0.00180001, indicating that the majority of unshielded neutrons were effectively attenuated by polyethylene. However, a peak in neutron count remained at lower energies, with a thermal neutron count of 0.025998. This necessitated the inclusion of boron-containing materials for thermal neutron absorption.
4. **Thermal Neutron Shielding with Boron Carbide:** Based on the results from the first two layers, the third layer was designed to shield thermal neutrons. The addition of 3 cm of boron carbide significantly reduced the neutron count rate to 0.000853831 at 0.5 MeV and 0.000357094 for thermal neutrons. This represents a substantial decrease in thermal neutron transmission compared to configurations without boron carbide, confirming its effectiveness in shielding thermal neutrons.
5. **Gamma-Ray Shielding:** Secondary gamma rays with energies below 10 MeV are generated during neutron shielding, necessitating additional shielding. Simulations showed that the maximum gamma-ray count rate occurred at 0.5 MeV. A thickness of 12 cm of iron was found to provide satisfactory gamma-ray shielding. Therefore, 12 cm of iron was selected as the fourth layer.

Summary: This study utilized the Monte Carlo method implemented in MCNP5 to investigate the neutron shielding performance of various materials and to identify an optimal neutron shielding scheme. The results indicate that a combination of 24 cm of iron, 8 cm of polyethylene, 4 cm of boron carbide, and 24 cm of iron provides an effective shielding solution. Compared to other material combinations, this configuration offers excellent shielding performance, low material cost, ease of transportation, and availability of raw materials. Given that 14 MeV neutrons are currently used in applications such as fast neutron radiography, neutron logging, and radiation breeding, the findings of this study are well-suited to meet the neutron shielding requirements of these applications.

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