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A method to optimize the shield compact and lightweight combining the structure with components together by genetic algorithm and MCNP code

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HIGHLIGHTS

- A method to optimize the shield combining the structure with components together was carried out.
- Six types of materials were presented and optimized.
- Geometry effect of four geometries used in practice has checked.

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ABSTRACT

To optimize the shield for neutrons and gamma rays compact and lightweight, a method combining the structure and components together was established employing genetic algorithms and MCNP code. As a typical case, the fission energy spectrum of ^{235}U which mixed neutrons and gamma rays was adopted in this study. Six types of materials were presented and optimized by the method. Spherical geometry was adopted in the optimization after checking the geometry effect. Simulations have made to verify the reliability of the optimization method and the efficiency of the optimized materials. To compare the materials visually and conveniently, the volume and weight needed to build a shield are employed. The results showed that, the composite multilayer material has the best performance.

1. Introduction

Radiation shielding is an important part of the nuclear facilities. For the facilities have abundant space, such as nuclear reactors and accelerators, the shield is quite simple because concrete is relatively inexpensive and could provide adequate shielding for the neutrons and gamma rays which are mainly considered during the shielding design. However, for the facilities whose space are limited, such as compact pressurized water nuclear reactor (Tunes et al., 2017), compact accelerator-driven neutron source (Hu et al., 2017) and some other compact systems or mobile devices, the shield becomes much more difficult. It must be compact, lightweight, and might be very specialized (Wielopolski et al., 2007). Even for the most experienced shielding designers, they may do not know whether their design is optimal in any sense. Thus, it is important to have a study on the shielding design for the compact systems and mobile devices.

In general, the method of shield designing is a "brute force" trial-and-error procedure which is tempered by experience (Schaeffer, 1973). However, optimization techniques using genetic algorithms, linear programming, sequential quadratic programming and transmission matrix methods (Guang Hu et al., 2017; Hu et al., 2008; Kebwaro et al., 2015; Leech and Rohach, 1972; Tunes et al., 2017) have gradually applied to improve it in recent years. Several composite materials and multilayer materials with excellent performance have presented in the studies, and these studies demonstrated that it is efficient to design the shielding material based on optimization algorithms.

However, there still exists a problem that the shields are almost designed by varying the thickness or component of the material alone. There lacks an integrated design of the shield combining the structure and components together (The "structure" means the thickness ratio and total thickness of the multilayer shielding material, the "components" means the components of the each layer). Moreover, due to the change of energy spectrum, the optimum thickness ratio of the multilayer material should be varied with its total thickness. But the previous studies are all tended to optimize it using a small thickness, and apply the solution to a larger thickness then. It is improper to do as that. Thus, it is necessary to carry out an effective method to design the shield compact and lightweight combining the structure and components together. This study exactly addresses this problem.

First, the shielding of neutrons and gamma rays are analyzed, and

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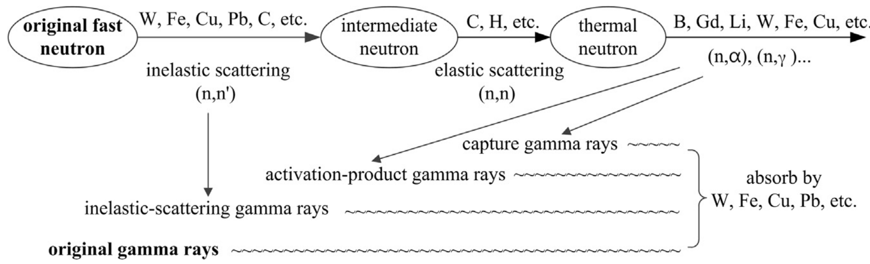

Fig. 1. Main interactions should be considered in the shielding of neutrons and gamma rays.

six types of materials are presented, then the calculation models and the method to optimize the shielding material are studied (Section 2). Second, the six types of materials are optimized, and comparisons between them with some conventional materials available are made (Section 3). The shortcomings and outlooks of this study are reviewed at last.

2. Methodology

2.1. Shielding principle of neutrons and gamma rays

The shielding principle of neutrons and gamma rays are based on the interactions between them and the materials, as shown in Fig. 1. For neutrons, the interactions include scattering and absorption. Objectively, all the interactions could occur in the whole energy range, but the main mechanisms to attenuate neutrons may vary with the energy and the material. The inelastic scattering dominates the fast neutron range, the elastic scattering dominates the medium energy range, and the capture reaction dominates the thermal energy range. Moreover, secondary gamma rays would be generated in the process of inelastic scattering and the reactions such as (n, γ), (n, α), (n, 2n), etc. It implies that the gamma rays should also be considered in the shielding of neutrons. For gamma rays, the interactions contain photoelectric absorption, Compton scattering and pair production. Thus, the shielding of neutrons needs materials contain both heavy and light elements, while the gamma rays only need heavy elements.

Obviously, to make a shield compact and lightweight, each of its compositions must be fully functioning and the elements undesirable (with drawbacks or useless) must be as low as possible. In this study, considering the cost of the material, the elements Fe, Pb, C, B and H are selected to make up the shield in the form of composite material and multilayer material. Among these elements, Fe and Pb are set as simple substances, while B and H are set as B_4C and polyethylene (PE) respectively. The PE is also the matrices of the composite shielding material.

As a typical case, the fission energy spectrum of ^{235}U (beam intensity is 10^{10} fission/s) which mixed neutrons and gamma rays was adopted in this study. It releases 2.407 neutrons (Watt fission energy spectrum) and 7.77 gamma rays every event. An empirical formula for the prompt gamma rays spectrum was employed (Schaeffer, 1973):

$$N(E_\gamma) = \begin{cases} 6.6 & 0.1 < E_\gamma \le 0.6\,MeV \\ 20.2\exp\ (-1.78E_\gamma) & 0.6 < E_\gamma \le 1.5MeV \\ 7.2\exp\ (-1.09E_\gamma) & 1.5 < E_\gamma \le 10.5MeV \end{cases} \quad (1)$$

In this study, calculations to design the optimal shielding are performed using the MCNP5 code and the ENDF/B-VI cross section set. Mode n p is used. The NCRP-38 (Rossi and Chairman, 1971) neutron flux-to-dose rate conversion factors and the 1977 ANSI/ANS (Battat, 1977) photon flux-to-dose rate conversion factors are used. To improve the calculation of the scored quantity, variance reduction techniques such as weight windows are used. 3×10^6 particles are simulated in the optimization process, and 2×10^8 particles are simulated in the other calculations. The calculation during optimization has a standard deviation less than 10%, while the others less than 5%.

2.2. Forms of the shielding material

In general, there have three forms of shielding material – single homogenous material, single composite material and multilayer material. Of which, each layer of the multilayer may also be composite materials. As mentioned previous, the single homogenous materials are not a good choice for the shielding of neutrons. Thus, this study only discusses the latter two forms.

For the multilayer materials, they utilize the material physically separate, that makes them maximize the role of each substance, and provide extra degrees of freedom for tuning the neutrons and gamma rays to energies where they can be effectively absorbed without excessive low energy tailing (Hong, 2002). For the composite materials, they can be formed into any shapes at one time, and the elements needed could be added into them easily. Thus, six types of shielding material are presented in this paper, as shown in Fig. 2. The structures of the materials are described below:

(a) Three-layer material, from left to right is Fe, PE and Pb respectively. The first layer Fe was set to attenuate the gamma rays, as well as slow down the fast neutrons to intermediate energy by inelastic scattering, the second layer PE was set to further moderate the neutrons to thermal energy by elastic scattering, and the last layer Pb was set to attenuate the secondary gamma rays and the original gamma rays.
(b) Three-layer material, from left to right is Fe, BPE and Pb respectively. The second layer BPE means a composite material consists of PE and B_4C. The B_4C was added to reduce the thermal neutrons and secondary gamma rays.
(c) Two-layer material, from left to right is Fe and a composite material consists of PE, B_4C and Pb.
(d) A block of composite material consists of PE, B_4C, Fe and Pb.
(e) Two-layer composite material both consists of PE, B_4C, Fe and Pb.
(f) Three-layer composite material all consists of PE, B_4C, Fe and Pb.

Because the reaction cross sections of neutrons and gamma rays are varied with the elements and energy, and different reaction has different energy losses, there may exists an optimal material for the shielding of specific neutrons and gamma rays. For the composite materials, it means an optimal component. For the multilayer materials, it means an optimal thickness ratio (may contains composite as well). Elbio Calzada (Calzada et al., 2011) has demonstrated that the optimum material composition is existed indeed by brute-force enumerate the shielding performance of all the components. In the same way, the optimal material thickness ratio should also exist for multilayer materials. Therefore, it is necessary to carry out a research about the method of optimization. The method may employ an optimization algorithms (such as genetic algorithms) and MCNP code. Considering large amounts of calculations are needed in the optimization process, and the time needed for the transport calculation by MCNP may be seconds even minutes (Intel i7–4790 CPU, 8 threads) per count, the calculation models should be studied before the optimization.

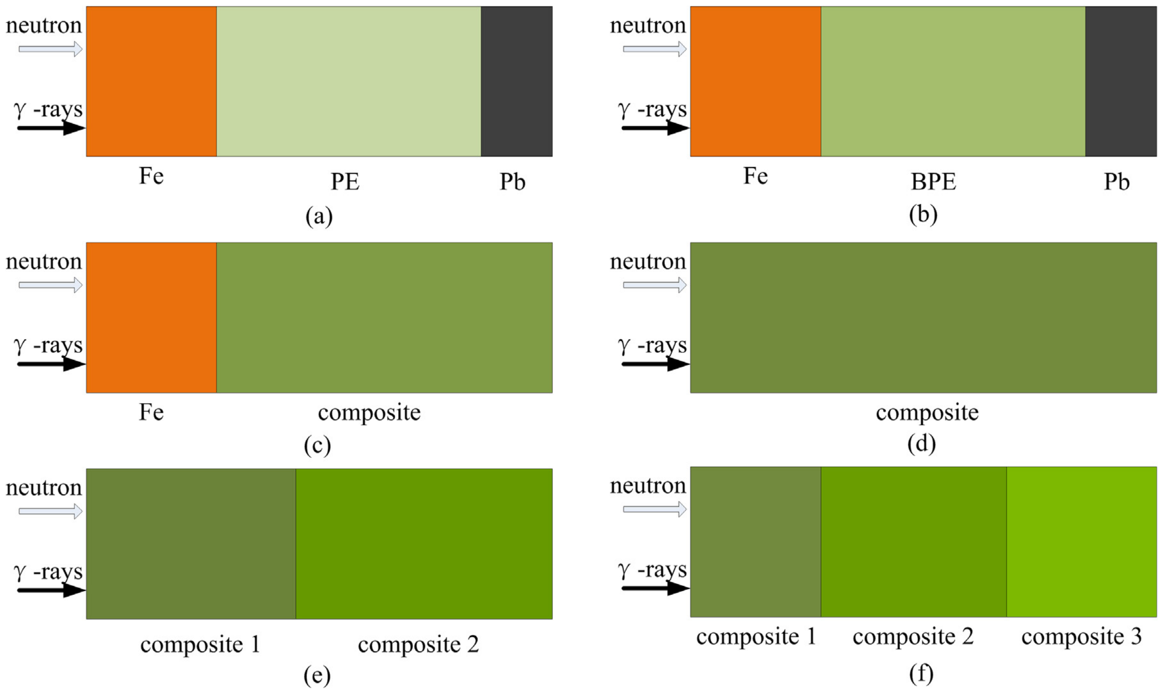

Fig. 2. Six types shielding material.

2.3. Calculation models

The shielding geometry in practice mainly contains four types: sphere, cylinder, cube and slab. To check the geometry effect, four geometries (Fig. 3) with material of PB202 (Lu and Chen, 1994) (developed by the Nuclear Power Institute of China, it shows good performance for the shield of neutrons and gamma rays) have examined. The fission energy spectrum of ^{235}U was adopted in the comparison. A point isotropic radiation source (neutron or gamma with fission energy spectrum of ^{235}U) is located at the center of the geometry in (a), (b) and (c), while it is located 10 cm to the left of the slab in (d). A series of point detectors (F5 tally card) are set at different distance to access the dose equivalent (locate right of the source, for the cylinder, the dose equivalent at the upside is smaller than that at right side).

The comparison in Fig. 4 shows that the effect of the geometry is small (less than 25%), and the total dose equivalent mainly contributed by neutrons in this case. When the distance is small, due to the scattering from the corners (for the slab, it is from the material extended), dose equivalent penetrated from sphere is the lowest, and the other three are almost the same (the difference among the four is quite small, less than 10%). When the distance becomes larger, the effect of scattering becomes smaller, and the dose equivalent penetrated decrease with the increase of shielding material thickness certainly, the dose equivalent penetrated from sphere becomes the largest.

Therefore, if the dose equivalent interested is near to the surface of the shield, the difference among the four geometries is small, and a material suit for the sphere would also suit for the others. If the dose equivalent interested is far from the surface of the shield, the spherical geometry performs worst with the same material thickness, and a material suit for the sphere would suit for the others as well. In addition, a

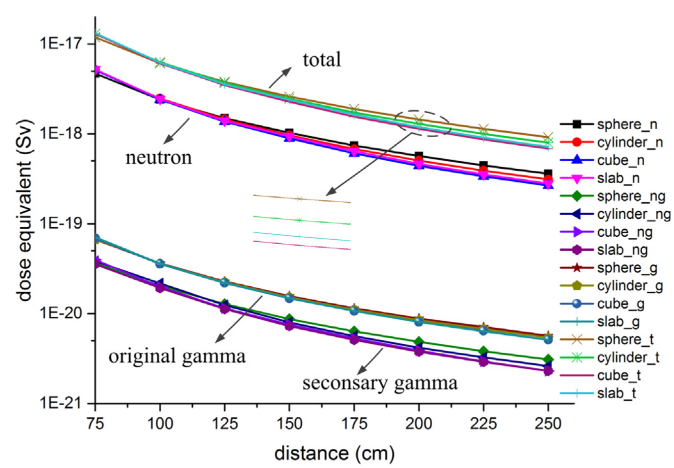

Fig. 4. Comparison among four types of geometries: dose equivalent at different distance (the out surface of the shield located position of 60 cm). The postfix n means neutron, ng means secondary gamma, g means original gamma, t means the total of all ($H_T = 2.407(H_n + H_{ng}) + 7.77H_g$).

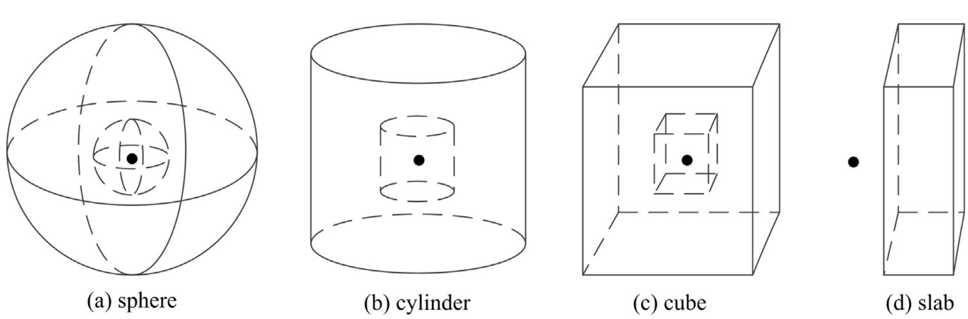

Fig. 3. Four modes used to check the effect of geometry. (a) The internal and external radius of the shell are 10 cm and 60 cm respectively; (b) The inner and outer radius of the cylinder are 10 cm and 60 cm respectively, also the half-height of the internal and external cylinder; (c) The sides of the internal and external cube are 20 cm and 120 cm respectively; (d) The thickness of the slab is 50 cm, the other two sides are both 4 m (a wall).

sphere is an idealized shielding geometry to make the simulations, combing with the surface detector, it can achieve better calculation accuracy with fewer particles. Thus, the spherical geometry and surface detector (F2 tally card) were adopted in the following optimizations.

2.4. Optimal design of the shielding material by genetic algorithm

The genetic algorithm (GA), which is based on natural selection, is widely used for solving both constrained and unconstrained optimization problems. It works on a population of individuals, and repeatedly modifies the potential solutions relying on bio-inspired operators such as mutation, crossover and selection. Over successive generations, the population "evolves" toward an optimal solution. In this study, a GA program called GENOCOP (Michalewicz and Janikow, 1996) developed by Michalewicz and Janikow was selected for optimization, it has excellent global search capabilities and optimization efficiency.

To design a multilayer shielding material compact and lightweight, the dose equivalent penetrated should be mainly considered because the optimum thickness ratio may vary with its total thickness. Moreover, the volume and weight should also be taken into account. In other words, the optimization is to make the weight and volume of the material as small as possible under the condition of meeting the specified dose equivalent (to make it easier finding the optimal solution, the target dose equivalent was set at $0.9H^*$ to H^*, as shown in formula (4)). The objective function of this multi-objective optimization problem can be written as follows:

$$f(X) = c_1 \cdot f_H(X) + c_2 \cdot f_M(X) + c_3 \cdot f_V(X) \tag{2}$$

Where

$$H_T(X) = H_n(X) + H_g(X) \tag{3}$$

$$f_H(X) = \begin{cases} \left|\frac{H_T - H^*}{H_T}\right| , & 0.9H^* \le H_T \le H^* \\ 1000 , & else \end{cases} \tag{4}$$

$$V(X) = \sum_{i=1}^{n} V_i \tag{5}$$

$$f_V(X) = \frac{V(X)}{V_0} \tag{6}$$

$$M(X) = \sum_{i=1}^{n} V_i \cdot \rho_i \tag{7}$$

$$f_M(X) = \frac{M(X)}{M_0} \tag{8}$$

So the optimization problem can be presented as follows:

$$\min f(X) \tag{9}$$

$$\text{s.t.} \quad \sum_{i=1}^{I} x_{1i} = 1, \quad \sum_{j=1}^{J} x_{2j} = 1, \quad \dots, \quad \sum_{k=1}^{K} x_{mk} = 1 \tag{10}$$

$$L_1 \le X_1 \le U_1, \quad L_2 \le X_2 \le U_2, \quad \dots, \quad L_m \le X_m \le U_m \tag{11}$$

where the equality constraints in (10) represent thickness ratios or components; The domain constraints in (11) represent the upper and lower bounds of the variables; X is the variable vector contains thickness ratios, components and total thickness; $f(X)$ is the total fitness function value; c_1,c_2 and c_3 are the weight coefficients; $H_T(X)$ is the total dose equivalent, Sv; $H_n(X)$ is the dose equivalent of neutron, Sv; $H_g(X)$ is the dose equivalent of gamma rays, Sv; $\rho(X)$ is the density of the material, g/cm^3; V and M are the volume and weight of the materials respectively, cm^3, g; V_0 and M_0 are the reference values to make the function dimensionless, cm^3, g; H^* is the target value of dose equivalent penetrated, Sv.

In this paper, weight coefficients was set at $c_1 = c_2 = c_3 = 1$. H^* was set at 2.5 μSv/h (6.94×10^{-10} Sv/s) which is a quarter of the occupational dose limit (10 μSv/h), assuming 40 h per week and 50 weeks per year (Zhong and Gohar, 2016). The reference values V_0 and M_0 are chosen according to the material PB202, set $V_0 = 2.57$ m^3, $M_0 = 8.78$ t (thickness of 75.0 cm to meet the H^* in spherical geometry).

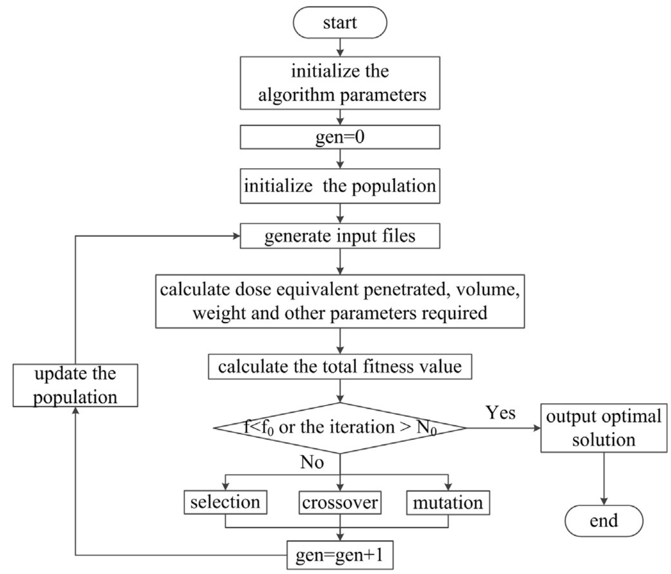

Fig. 5. Flow chart of the program employ genetic algorithm.

The steps in the GA optimization are presented in Fig. 5. First, initialize the parameters, such as population size, max generation and selective pressure. Second, generate the input files according to the parameters, and run the corresponding codes (by MCNP). Then get the volume, weight and dose equivalents every generation in each count, and calculate the total fitness value. Third, update the population employ the selection, crossover, and mutation operation of GA, and update the input files simultaneously, the optimal solution will be found after successive generations.

3. Optimal design results

In order to find the optimal shielding material, the domain constraint of each variable was set at 0–1 (the total thickness was set at 0–100 cm), the population size was set at 50–200 according to the number of variables (about 10 *Nvar), the cumulative probability distribution q was set at 0.1–0.3 according to the population size (higher q values provide stronger selective pressure), and the number of generations was set at 100 after several trials. To get the solutions in a reasonable time, appropriate range protection (2 m away from the source) was adopted to lower the shield thickness.

By running the program and adjusting the parameters, the six types of shielding material presented in Section 2.2 were optimized (aim at the fission energy spectrum of 235U), as presented in Table 1.

To compare the materials visually and conveniently, the volume and weight needed to build a shield are employed, and a parameter ξ_i which contains volume and weight was used to evaluate the performance of the materials.

$$\xi_i = M/M_0^i + V/V_0^i, \quad i = 1, 2, 3, 4 \tag{12}$$

The reference values M_0^i and V_0^i are also chosen according to the material PB202, and they are vary with the geometries (with a same thickness of 75.0 cm as previous). i = 1, 2, 3, 4 represent the geometry of sphere, cylinder, cube and slab respectively.

It can be noticed, for the material FESa and FESb, the main difference lies in the second layer. Some B_4C was added in the FESb, it significant reduced the thermal neutrons and secondary gamma rays, and

Table 1
The optimized shielding materials. The first column is the name of materials, where the symbol "FES" means the material was designed aim at the fission energy spectrum, the symbol "a", "b", …, "f" means the types of material shown in Fig. 2. The second column is the number of the layers. The T_n is the thickness of the layers, and T_{total} is the total thickness needed to meet the dose equivalent H^*. The V and M are the volume and weight of the shield respectively. The spherical geometry (the internal radius is 10 cm) was adopted.

Material	Layer No.	Component / wt%				Density /g cm^{-3}	T_n /cm	T_{total} /cm	V /m^3	M /ton	ξ_1
		Fe	PE	B_4C	Pb						
FESa	1	100				7.87	23.17	72.88	2.38	13.1	2.42
	2		100			0.95	36.85				
	3				100	11.34	12.86				
FESb	1	100				7.87	21.67	67.34	1.93	7.09	1.56
	2		54.89	45.11		1.32	40.42				
	3				100	11.34	5.25				
FESc	1	100				7.87	20.03	64.52	1.73	5.36	1.28
	2		22.38	18.13	59.49	2.78	44.49				
FESd	1	50.99	12.07	15.79	21.15	3.66	66.15	66.15	1.85	6.76	1.49
FESe	1	61.14	2.93	8.88	27.05	5.97	32.75	64.82	1.75	4.65	1.21
	2	17.50	38.56	18.71	25.23	1.91	32.07				
FESf	1	78.40	4.26	3.43	13.91	5.87	29.29	64.61	1.74	4.55	1.20
	2	34.90	14.74	21.54	28.82	3.22	10.21				
	3	13.48	42.45	13.57	30.50	1.84	25.11				

lead to a thinner thickness of Pb needed. So the volume and weight of FESb are both much smaller than those of FESa.

Follows, merge the latter two layers of FESb, the material FESc was obtained. The composite consists of PE, B_4C and Pb could moderate neutrons, absorb neutrons, and attenuate gamma rays simultaneously. Considering the weight of sphere (cylinder and cube) would decrease rapidly with the smaller density of the outer layer material, the volume and weight of FESc are both further smaller than those of FESb.

Then, merge the layers of FESc furthermore, the material FESd which is a block of composite material was obtained. It can be treated as an optimized composite material, while the material FESb is an optimized multilayer material. As can be seen, the optimized composite is a bit better than the optimized multilayer FESb, but worse than the multilayer FESc. That is to say, a reasonable multilayer is better than a block of composite material.

Thus, divide the composite FESd into two parts, the material FESe which is a two-layer composite was obtained. Its structure is similar to FESc, since the composite could better serve the specific neutrons and gamma rays by adjusting its composition, the performance of FESe become a bit better than that of FESc.

Furthermore, divide the composite FESd into three parts, the material FESf who has more layers than FESe was obtained. It implies that FESf has larger degree of freedoms than FESe to adjust its components according to the energy spectrum of neutrons and gamma rays. As shown in Table 1, the former two layers contain more Fe to slow down the fast neutrons as well as attenuate the gamma rays, the latter two layers have more PE to slow down the intermediate neutrons, and the last layer has more Pb to attenuate the secondary gamma rays and original gamma rays. Because of its more scientific and reasonable structure, it is further improved compare with the previous materials.

According to the analysis above, the composite multilayer material as FESf has the best performance. Furthermore, it is conceivable that the gradient material is a most suitable material for a specific application, since its composition could vary with the spectrum of the radiation. However, it would be difficult to synthesize, and the type "f" is an extreme situation of it. In addition, if there has too many layers, it would difficult to achieve the optimal solution due to its too many variables.

To examine the applicability of the optimized materials in other geometries, the four geometries with these materials were checked, the results are listed in Table 2. It can be seen, they have all achieved the target value of dose equivalent H^*. That is to say, they can be built as all the four geometries. Comprehensive considering the dose equivalent, volume and weight of the shield, the composite multilayer material as FESf is still a better choice to build a shield in the all four geometries.

Table 2
Comparison of the optimized materials: dose equivalent (2 m away from the source, μSv/h) and ξ_i (contains volume and weight) in the four geometries. Point detector was used.

Material	Sphere		Cylinder		Cube		Slab	
	H	ξ_1	H	ξ_2	H	ξ_3	H	ξ_4
FESa	2.49	2.42	2.22	2.42	2.11	2.45	1.55	2.39
FESb	2.49	1.56	2.39	1.56	2.21	1.57	1.78	2.01
FESc	2.50	1.28	2.45	1.28	2.37	1.29	2.06	1.96
FESd	2.50	1.49	2.17	1.48	1.84	1.50	1.76	1.83
FESe	2.50	1.21	2.38	1.21	2.00	1.22	2.29	1.87
FESf	2.49	1.20	2.39	1.19	2.12	1.21	2.04	1.84

To further illustrate the efficiency of the optimized materials, several materials available (Table 3) were compared. The spherical geometry and surface detector as previous were adopted. The volume and weight of these materials needed to meet the dose equivalent H^* are listed in Table 4. It can be seen, the optimized materials are generally better than the materials compared. Additionally, it demonstrates the reliability and consistency of the optimization applied methodology in this work.

4. Conclusions

Thus far, the method to optimize the shield compact and lightweight combining the structure with components together for neutrons and gamma rays was established employing genetic algorithms and MCNP code. The factors need to be considered and steps to reach the optimization objective were presented as well. Geometry effect has checked by compare the four geometries (sphere, cylinder, cube and slab) used in practice, it showed that the geometry effect is small, and a material suit for the spherical geometry would also suit for the other three. Six types of materials have presented and then optimized by the method. Simulations have made to verify the reliability of the optimization method and efficiency of the optimized materials. To compare the materials visually and conveniently, the volume and weight needed to build a shield are employed. The results showed that, the composite multilayer material as type "f" has the best performance. For the single composite material (type "d") and simple multilayer material (type "b"), the optimized single composite is a bit better in this case. The

Table 3
Composition of the shielding materials compared (weight fraction).

Material	Density	Fe	O	Ca	H	C	B	Pb	Minor elements
Hormirad (Fillol et al., 2008)	3.99	60.8	31.26	4.36	0.44	0.04	–	–	Si, Mg, P, Ti, Al, K, Mn, V, S, N, Na
Heavy concrete (Calzada et al., 2011)	4.68	79.06	14.57	4.27	0.46	–	0.34	–	Si, Mg, Al
Mixture (Calzada et al., 2011)	5.14	91.15	–	–	0.92	6.03	1.90	–	–
PB202 (Lu and Chen, 1994)	3.42	–	–	–	2.73	16.49	0.78	80.00	–

Table 4
Volume and weight the materials needed.

Material	T_{total} /cm	V /m^3	M /ton	ξ_1
Hormirad	102.35	5.94	23.7	5.01
Heavy concrete	89.79	4.16	19.5	3.84
Mixture	66.1	1.84	9.47	1.79
PB202	75.0	2.57	8.78	2.00
FESf	64.61	1.74	4.55	1.20

results of research can be wide applied to the practices of nuclear science and technology.

However, this study only considered the properties of volume and weight, while the mechanical properties, thermal properties and radiation resistance were ignored. To further improve the design method and obtain more ideal materials, those properties should be taken into account in the future research. And some other optimization algorithms should be studied to find an algorithm with better efficiency. The related experiments should be carried out in the future research as well.

Acknowledgements

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