Investigation of Nanoparticle Effect on Radiation Shielding Property Using Monte Carlo Method

Huseyin Ozan Tekin*[1], Vishwanath P. Singh[2], Umit Kara[3], Tuğba Manıcı[4], Elif Ebru Altunsoy[5]

[1]Uskudar University, Vocational School of Health Services, Radiotherapy, İstanbul, Turkey
Tel: +902164002222 Fax: +902164741256, huseyinozan.tekin@uskudar.edu.tr
[2] Karnatak University, Department of Studies in Physics, Dharwad, India
Tel: +9108382264225 Fax: +9108382262114, kudphyvps@rediffmail.com
[3] Suleyman Demirel University, Vocational School of Health Services, Medical Imaging, Isparta, Turkey
Tel: +902462110000 Fax: +902462370431, umitkara@sdu.ede.tr
[4]Uskudar University, Medical Radiation Research Center (USMERA), İstanbul, Turkey
Tel: +902164002222 Fax: +902164741256, tmanici@gmail.com
[4]Uskudar University, Medical Radiation Research Center (USMERA), İstanbul, Turkey
Tel: +902164002222 Fax: +902164741256, elifebru92@gmail.com
*Corresponding author / İletişimden sorumlu yazar

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Abstract

Radiation protection and choice of appropriate materials in the areas of medical and industrial applications has become one of the major research topics. In this study, the increment in mass attenuation coefficients by doping of nano-sized barite (BaSO4) into the lead (Pb) have been investigated. The validation of generated MCNPX simulation geometry is provided by comparison with the previous experimental and theoretical studies. This generated geometry was used for the definition of nano-$BaSO_4$ into lead material and calculations. It was found that nano-$BaSO_4$ doped lead increased the amount of radiation absorbed in the material inside and as a result of which affected the radiation attenuation properties of material. This study also showed that MCNPX is an effective code on nano size studies and standarised geometry can be useful for further investigations.

Keywords — Radiation Shielding, Mass Attenuation Coefficient, Monte Carlo Method, Nanoparticles, MCNPX

Radyasyon Zırhlama Özelliğinde Nanoparçacık Etkisinin Monte Carlo Metodu Kullanarak İncelenmesi

Özet

Radyasyondan korunma ve uygun malzeme seçimi medikal ve endüstriyel radyasyonun kullanıldığı alanlarda başlıca araştırma konularından bir tanesi haline gelmiştir. Bu çalışmada, kurşun (Pb) içerisine nano boyutlarda barit ($BaSO_4$) katkısı yapılarak kütle zayıflatma katsayısında meydana getirdiği artış incelenmiştir. Oluşturulan MCNPX simülasyon geometrisinin validasyonu önceki deneysel ve teorik ölçümler ile sağlanmıştır. Oluşturulan bu geometri nano $BaSO_4$ parçacıklarının kurşun malzeme içerisine tanımlanmasında ve hesaplamalarda kullanılmıştır. Sonuç olarak nano boyutlarda kurşun içerisine katkılanan $BaSO_4$ nanoparçacıkları kurşunun kütle zayıflatma katsayısında bir artışa sebep olmuş, malzeme içerinde soğurulan radyasyon miktarı artmış ve malzemenin radyasyonun zayıflatma özelliklerini etkilemiştir. Bu çalışma ayrıca MCNPX kodunun nano boyutlardaki çalışmalarda etkili bir program olduğunu ve standartize edilen bu geometrinin gelecek çalışmalar için kullanılabilirliğini göstermiştir.

Anahtar Kelimeler — Radiation Shielding, Mass Attenuation Coefficient, Monte Carlo Method, Nanoparticles, MCNPX

1 Introduction

In the recent years, the use of the radiation in the various energy ranges has been increased in different fields, like medical, industrial, agriculture, etc. To forestall radiation staff and population exposure to ionization radiation, public and working areas should be shielded and protected. For this reason, investigations and studies on radiation attenuation properties and designs of new complex materials as an attenuator material have been increasing in the field of radiation protection.

On the other hand, direct and in-direct scattered radiation can be hazardous for the people. The mentioned potential rish are overcome by applying three main fundamental concepts shielding, distance and time. The first of those processes namely shielding commonly depending on gamma-ray energy and price of material. The attenuation features of radiation for a spesific target environment are required to determine the amount of shielding necessary [1]. The mass attenuation coefficient (μ_m) is one of the most important features for characterizing the penetration and diffusion of gamma-rays in target material [2]. The μ_m is a density independent coefficient and determined for target attenuator material by using the transmission method by Lambert-Beer law which is formulated as $\mu_m \cdot x = \ln (I_0/I)$. Where I_0 and I are the incident and attenuated photon intensity, respectively. The μ_m ($cm^2.g^{-1}$) is the mass attenuation coefficient and x is the thickness of the slab.

On the other hand, the effectiveness of radiation shielding is described in terms of the half value layer (HVL) and the tenth value layer (TVL) of a target attenuator material. The HVL is the thicknesses of attenuator that will reduce the incident radiation amount to half value, and the TVL is the thicknesses of an absorber that will reduce the incident radiation amount to one tenth value of its original intensity [3].

Abilities of MCNPX code have been studied by considering the different applications in the field of radiation. Investigation of detector efficiency and using in different applications has been studied by Akkurt et.al [5]. Capability of MCNPX for dose distribution has been studied by Tekin et.al [6]. Investigation of backscattered dose in a computerized tomography (CT) facility by using MCNPX code has also been studied Tekin et.al [7].

On the other hand, MCNPX code has been used during different nanoparticle researches. The effect of gold nanoparticle on dose enhancement has been studied by Abolfazli et.al [8]. Effects of WO_3 particle size in WO_3/epoxy resin radiation shielding material has been studied by Dong et.al [9]. Dose enhancement in brachtherapy in the presence of gold nanoparticle and modelling by using MCNPX code has been studied by Ghorbani et.al [10].

The theoretical, experimental and simulation investigation on interaction of gamma-ray with elements, composites materials and compounds are found in various literatures in recent years. The compounds and composite materials cover variety of containing low-Z to high-Z elements useful for dosimetry and shielding, respectively. The effectiveness for shielding of these materials can be found elsewhere. However, gamma-ray interaction with nanoparticles and their effect with doping of elements couldn't be found in the literature so far. Therefore, this study aimed to determine the effect of doping nano-$BaSO_4$ inside of the lead attenuator material and evaluate to changes of attenuation parameter of lead attenuator material using Monte Carlo method.

2 Material and Method

2.1. MCNPX code and simulation methods

MCNPX is a general purpose radiation transport code for modeling the interaction of radiation with materials and also tracks all particles at all energies. MCNPX is fully three-dimensional and it utilizes extended nuclear cross section libraries and uses physics models for particle types [4].

In this study, MCNPX simulation process can be divided into two steps. As a first step, we created a simulation geometry by using the physical parameters of simulation equipments to verify the validation of our input file. The mass attenuation coefficients of lead (Pb) have been calculated and compared with XCOM data [11]. The total simulation geometry is seen in fig.1 and as it can be seen, one cylindrical 3×3 inch NaI (Tl) detector of height in crystal 7.62 cm and diameter 7.62 cm and with a mono-energetic isotropic point source. Also, the source and detector assembly was shielded by lead blocks.

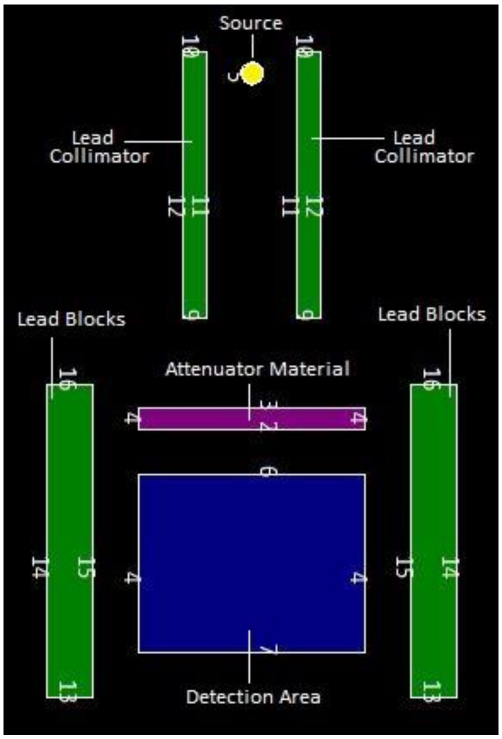

Figure 1. Simulation geometry of valiation calculations

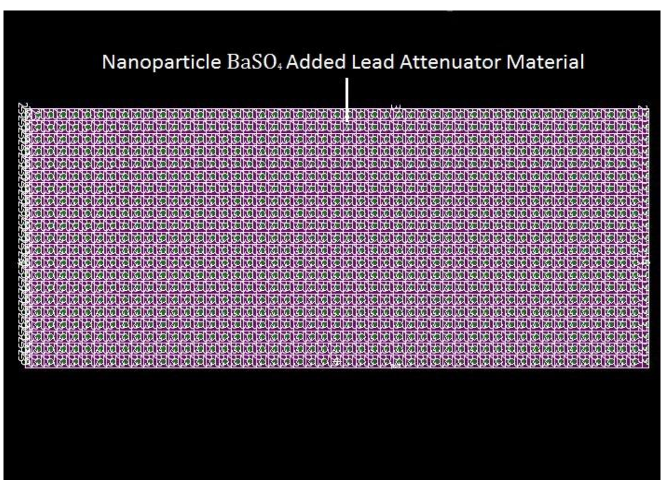

Figure 2. Schematic view of nano-$BaSO_4$ in attenuator material

Fig.1 shows the MCNPX simulation geometry of valiation calculations. As a second step of the this study, nano-$BaSO_4$ have been introduced into lead attenuator material in MCNPX input file.

2.2. Definiton of nanoparticles in MCNPX code

In this study, each nano particle voids have been defined by using the lattice (LAT) and universe (u) features of MCNPX code. The definition of each one nanoparticle into the attenuator material has been considered for 100 nm diameter of $BaSO_4$ sphere geometry into an edge of 2 μm cube. The lead attenuator material has been modeled as 8x8x2 cm cube so $1,6x10^{13}$ nano-BaSO4 has been dopped inside of lead. The schematic view of nano-$BaSO_4$ added target can be seen in Fig.2 with defined sphere nano geometries into cubes.

Gamma-ray source, lead (density=11,34 g/cm^3) collimator, attenuator target material, detection area have been defined in cell card, surface card and data card sections of MCNPX input by considering different variable such as CEL, ERG, DIR, POS, and PAR. The geometric center of detection cell has been considered for location of point source. During the Monte Carlo simulation, each variable has different abilities. In our study, variables commanded source cell, energy, direction, source position respectively. On the other hand, one of important definition is material specification by considering atomic number, mass number and density (d) for pure elemental materials and atomic number, elemental mass concentrations and density for compounds or mixtures. By considering these variables, we defined firstly the pure lead attenuator material and secondly $BaSO_4$ nanoparticles added lead attenuator material in input file respectively. In the MCNPX simulation process 10^6 photons were used as a number of particle.

To obtain absorbed dose amount in detection area, energy deposition mesh tally (F6) has been used as a mesh tally. This type of tally in MCNPX scores energy deposition data in which energy deposited per unit volume from all particles is included. MCNPX calculations were done by using Intel® Core ™ i7 CPU 2.80 GHz computer hardware.

3 Results

3.1. Validation of MCNPX

To confirm the validation of our generated MCNPX input file, we calculated the mass attenuation coefficients of lead by using our input file and compared the results with standart XCOM data. During the validation study the error rate was less than %1 in output file. On the other hand, standard deviations between our results and XCOM data have been calculated and pointed out in Table 1.

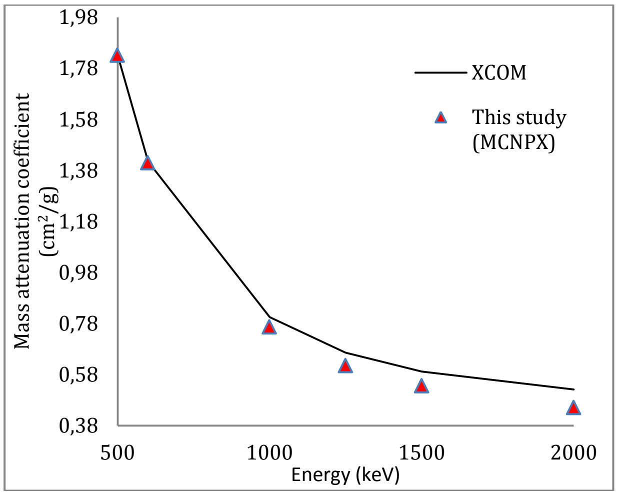

Figure 2. Comparison of MCNPX results versus XCOM data

Table 1. Mass attenuation values of lead (density=11,34 g/cm^3) obtained from XCOM and MCNPX and standart deviation values between results

Energy (keV)	XCOM	This Study (MCNPX)	Standard Deviation ($D=E_a-E_b/E_b$ x100%)
500	0,1614	0,1611	0,1862
600	0,1248	0,1243	0,4022
1000	0,0710	0,0701	1,2838
1250	0,0587	0,0582	0,8591
1500	0,0522	0,0516	1,1627
2000	0,0460	0,0456	0,8771

Table 2. Mass attenuation coefficients (cm^2/g) of lead and nano-$BaSO_4$ added lead.

Energy (keV)	Lead (Pure)	Lead (nano-$BaSO_4$)	Rate of increase (%)
500	0,1614	0,1637	1,4609
600	0,1248	0,1254	2,7386
1000	0,0710	0,0712	3,0495
1250	0,0587	0,0587	4,8364
1500	0,0522	0,0524	5,9179
2000	0,0460	0,0462	5,5463

As it can be seen from Fig.2, we achieved a significantly good agreement between XCOM and MCNPX data. The standard deviation rates obtained in the range of 0,1862 to 1,2838. Entire data comparison between XCOM and MCNPX have been obtained in good agreement and standart deviation rates have been pointed out as well. Thus, modeled MCNPX simulation input has been confirmed as a validated input and then considered as a standard and usable simulation input for the second step of this study namely definition of nanoparticles in MCNPX code.

3.2. Effect of $BaSO_4$ nanoparticles on attenuation properties of lead (Pb)

The validated simulation input has been used to investigate the effect of nano-$BaSO_4$ in lead attenuator material. The mass attenuation coefficients of pure lead and $BaSO_4$ nanoparticles added lead have been calculated at photon energies of 500, 600, 1000, 1250, 1500, 2000 keV and the results were compared.
The calculated results and rates of increase for each energy tablulated in Table 2. It is clearly seen from the Table 2 that adding of nano-$BaSO_4$ affected the increasing rate of the mass attenuation coefficients in different rates on different energies. As the energy increases, effect of the nano-$BaSO_4$ has been observed increasingly. Somehow, the maximum rate of increase has been obtained at 2000 keV as % 5,5463. During the calculations the error rate was less than %1 in output file.

4 Discussion and Conclusion

The selection of attenuator materials for radiation shielding mostly depends on the amount of radiation, type of radiation and energy of radiation. In previous studies, Akkurt et al. experimentally reported that attenuation properties for $BaSO_4$ added materials are higher than regular sample [12]. Nowadays, studies on nano-sized particles increasing rapidly. Kim et. al reported that attenuation of gamma photon was enhanced ~%75 for nano-tungsten (W) [13]. Different possible features nano-$BaSO_4$ have been studied in literature. The possiblity of nano-$BaSO_4$ for being novel antimicrobial additive to pellet have has been studied by Aninwene et. al [14]. In this study, we investigated the possible effect of nano-$BaSO_4$ on radiation attenuation properties of conventional shielding materials. During the first step of our study, validation of input file has been provided and a good agreement between XCOM standart data and our result has been achieved. Thus, standarted input file has been used for effect investigation of nano-$BaSO_4$ on lead attenautor material. The results showed that attenuation of radiation was enhanced with nano-$BaSO_4$. The mentioned enhancement has been observed in different rates depending on the energy.

Monte Carlo results showed that effect nano-$BaSO_4$ on attenuation has been enhanced by increased energy value. The maximum increasing rate of the mass attenuation coefficients for an energy value has been obtained on 2000 keV and the mass attenaution coefficient value has been increased as %5,5463. The error rates have been obtained less than %1 during all the calculations. Somehow, nano-$BaSO_4$ effected the attenuation properties of lead in each energy ranges. Apart from the producibility of mentioned composite nano-$BaSO_4$ lead material, it can be concluded that effect of nano-sized $BaSO_4$ with regular distribution in target material can be used for better shielding in different application fields such as industiral and medical radiation areas. On the other hand, this study showed that Monte Carlo method can be applied for possible future studies on nano-sized particles and MCNPX is a strong code for mentioned studies. The standardised geometry for Monte Carlo simulation can be used in further studies.

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