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# A comparatıve study on shielding properties of some composite materials by MCNPX code

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The radiation mass attenuation coefficients of composite material samples as shielding materials have been calculated at 356, 511, 662, 1173, 1274 and 1332 keV photon energies by using general purpose Monte Carlo code MCNPX (version 2.6.0). The obtained numerical results agree well with experimental and standard XCOM data. As a result, the maximum values of mass attenuation coefficients are found for D1 and D2 composite material samples. It can be concluded that, new generation composite materials can be alternative shielding materials against gamma-ray radiation and Monte Carlo method can be employed for similar material investigations as an alternate tool for assessment.

**Keywords:** Mass attenuation coefficients, Polymer composites, Monte Carlo

The use of different types of materials for shielding applications is increasing day-by-day for industries, agriculture, space, medical, reactors, accelerators, etc, for reduction of exposure to occupational worker, patient, etc. The choice of shielding materials is highly dependent upon the requirement for exposure rate reduction, type of source, space constrains and final cost effective analysis. Nowadays, lead is common and very useful material in the field of nuclear engineering for shielding applications. However, the toxic properties and cost of lead have led to the investigation of alternative shielding materials and various investigations and products are readily available. The polymer composite materials which are harmless to the environment and non-toxic are suitable alternate with both personal and material shielding, efficiently. In general, experimetal studies requires not only materials, radiation sources and experimental setup of very high financial budget but also radiation exposure to involved personnel. However, mathematical simulation methods for investigation of radiation interaction is found less time consuming, radiologically safer, cost suitable and applicable for desired energy of radiation. It is found that, Monte Carlo simulation is suitable method for investigation of radiation interaction with materials in various literature elsewhere[1-11]. The radiation mass attenuation coefficient is basic property of a material for photon interaction to indicate interaction and shielding effectiveness. The mass attenuation coefficient of an element is found to be constant at particular photon energy, while mass attenuation coefficient of a compound or mixture depends upon chemical composition of elements[12]. On the other hand, another radiation shielding parameters such as the linear attenuation coefficient, half-value layer thickness (HVL), tenth-value layer (TVL) thickness and effective atomic number ($Z_{eff}$) are derived parameters from the mass attenuation coefficient. Previously, the shielding parameters of recent composite materials has been studied by Erol *et al*.[13]. But the computational simulation studies for photon interaction couldn’t be found in the literature. This has encouraged us to set a simulation setup to investigate the attenuation properties of those materials and validate the MCNPX (version 2.6.0) code. Therefore, this study aimed to investigate the mass attenuation coefficients of different types of composite materialsusing MCNPX (version 2.6.0) code at 365.5, 511, 661.6, 1173.2, 1274 and 1332.5

keV photon energies and generate a standard Monte Carlo simulation setup. The obtained results were compared with previous experimental and standanrd XCOM[14] data. The present paper using standard simulation geometry for MCNPX (version 2.6.0) code would be very useful for further studies of photon interraction with various types of composite materials for gamma shielding applications.

## Experimental Section

### Mass attenuation coefficient

In general, nearly all the material types can be used for shielding of gamma-ray, if they utilized in a particular material thickness. Somehow, the radiation attenuation properties of materials are highly dependent upon the density of the shielding material. For monochromatic gamma-ray, the intensity reduces as the photon beam propagates through the shielding material according to the Lambert-Beer law by following equation[15]:

$$I=I_0 \exp^{(-\mu t)} \qquad \text{... (1)}$$

where $I_0$ is the incident intensity of radiation, t is the path length, and μ is the linear attenuation coefficient of shielding material. The linear attenuation coefficient depends on the elemental or composition chemical of the sample. Due to linear attenuation coefficient depends on the density, an information which is independent of the density (μ/ρ) of the material is needed. This density independent information is called the mass attenuation coefficient and its unit is $cm^2/g$. The term of mass attenuation coefficient (μ/ρ) is the one of the significant parameter to evaluate the shielding properties of investigated attenuator materials. The mass attenaution coefficient can be obtained by dividing the linear attenuation coefficient (μ) by density (ρ) of studied shielding material. On the other hand, the radiation mass attenuation coefficient (μ/ρ) of a shielding material at a certain energy is the sum of the products of the weight fraction and the mass attenuation coefficient of the element i at that energy namely:

$$\mu / \rho = \sum_i w_i (\mu / \rho) i \qquad \text{... (2)}$$

where $w_i$ and (μ/ρ)i are the fractional weight and the total mass attenuation coefficient of the $i^{th}$ constituent in the mixture shielding material sample.

### MCNPX code

The general purpose Monte Carlo N-Particle Transport Code System-extended (MCNPX) version 2.6.0 (Los Alamos national lab, USA) code was applied to determine the mass attenuation coefficients of different types of composite materials. MCNPX is a Monte Carlo code designed to simulate various physical interactions over abroad energy range. MCNPX is fully three-dimensional and uses extended nuclear cross-section libraries and physics models for the different types of particles[16]. In this study, the gamma ray sources were defined in the mode card of the MCNPX input file as isotropic point sources at photon energies of 356, 511, 662, 1173, 1274 and 1333 keV. Likewise, each polymer composite shielding materials have been defined in MCNPX input file considering their elemental mass fractions. The elemental compositions and mass fractions can be seen in Table 1, respectively. As it can be seen from Table 1, each polymer composite material sample has different elemental mass fractions.

The required information in MCNPX input file can be ordered as; definition of the problem geometry, definition of the materials with their chemical composition and the definition of the radiation source structure. Moreover, it is also required to define the results that desired from the calculation. The geometry of simulation is constructed by defining cells. Each cells in simulation are bounded by one or more geometric surfaces. In the present investigation, square prism geometry was employed for the modeling of each antibacterial sample. The edge lengths of this square prism geometry are defined as 5 cm while the axial z-length is defined for each simulation in different sizes because it is the thickness of the polymer composite material sample. The inside of modeled square prism has been considered as a cell in input file. For each calculation, this cell is modeled as a different composite material with the different elemental mass fraction which given in Table 1.

The total simulation geometry of the present investigation for the mass attenuation coefficient calculations can be seen in Fig. 1. In addition, a cross-sectional screenshot of the MCNPX Monte Carlo code can be seen in Fig. 2. To obtain the absorbed dose amount in the detection field, the average

Table 1 — Elemental massfractions of polymer composite materials (%)

| Polymer Composite Material ID | WC | $B_4C$ | HDPE |
|---|---|---|---|
| D1 | 50 | 20 | 30 |
| D2 | 50 | 10 | 40 |
| D3 | 0 | 20 | 80 |
| D4 | 0 | 0 | 100 |

F4 flux tally was employed. This type of tally in MCNPX scores the average flux in a point or cell.

Moreover, a total of $10^8$ particles were tracked (the NPS variable). The analysis of recent investigation was performed using the the D00205ALLCP03 MCNPXDATA package is comprised of DLC-200/MCNPDATA cross-section libraries. This library typically extends ENDF/B-VI data from 20 MeV to 150 MeV. The MCNPX calculations were performed using an Intel® Core ™ i7 CPU 2.80 GHz computer.

## Results and Discussion

The mass attenuation coefficients of the different polymer composite shielding materials against photon energies of 356, 511, 662, 1173, 1274 and 1333 keV were investigated using MCNPX code, and the results are shown in Fig. 3. It is to be noted that the mass attenuation coefficients of each polymer composite material decrease with increasing photon energy, with the largest at 1333 keV. The behaviour of the variation of the mass attenuation coefficients

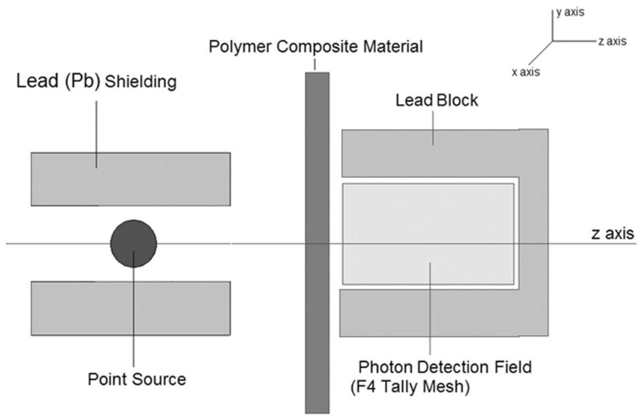
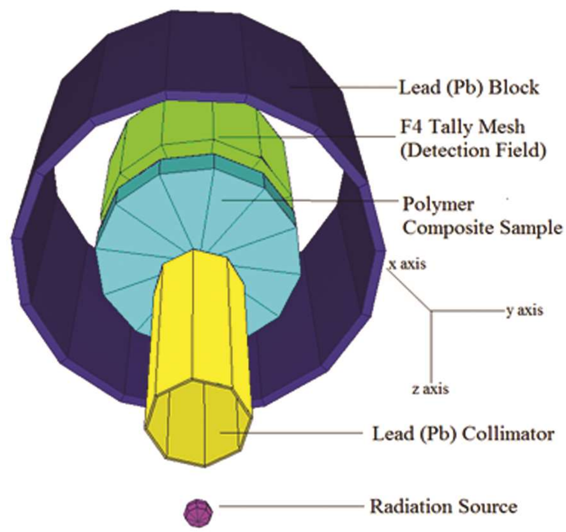



Fig. 1 — Total simulation geometry of the simulation of polymer composite materials




(a) (b)

Fig. 2 — The screenshot of MCNPX simulation setup

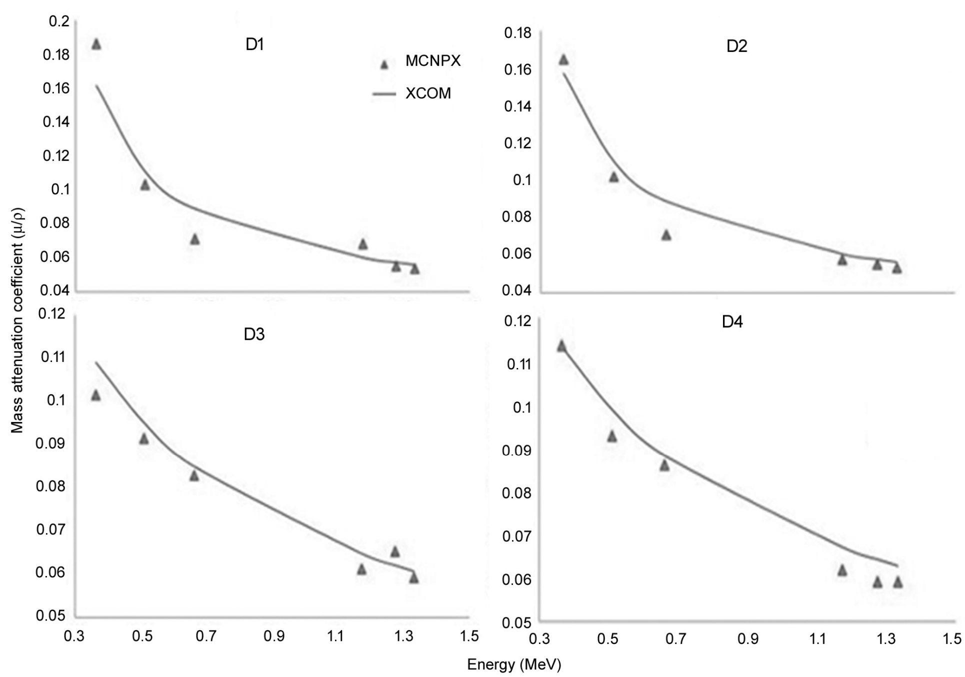



Fig. 3 — Comparison of MCNPX and XCOM results

with photon energy can be explained by photon interaction processes (e.g. the photoelectric effect, Compton scattering and pair production) in low, intermediate and high energy photon regions using the atomic number of the elements and the photon energy. It can be clearly seen that D1 and D2 polymer composite samples displays a higher mass attenuation coefficient at all energies. This can be due to higher amount of $B_4C$ inside the D1 and D2 polymer composite samples.

The results of the present investigation for the mass attenuation coefficients of polymer composite materials are comparable with experimental values by Erol *et al*. Therefore, validation of our Monte Carlo simulation setup can be considered. Therefore, the standard input file can be useful for further similar investigations especially with polymer composite materials. In addition, a slight difference between the XCOM and the MCNPX mass attenuation coefficient values was observed. This may be due to deviations from the narrow-beam geometry in the source–detector geometry, statistical parameters such as counting quantity.

## Conclusion

In the present work, MCNPX (version 2.6.0) code has been used for investigation of photon shielding characterizations of various composite polymer materilas. The μ/ρ, have been calculated at six photon energies. The variation of these paeameters was discussed in terms of both photon energy and concentration. It can be concluded that wolfram carbide□doped boron carbide polymer composite could be employed for shielding of gamma ray applications. This study showed that, shielding parameters of polymer composite systems can be investigated using Monte Carlo simulation. Therefore, it can be also concluded that modeled and validated standard MCNPX geometry and given simulation details can be useful for scientific community since the radiation shielding properties of different type of polymer composite materials being researched by Monte Carlo simulation method, frequently.

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