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Monte Carlo Simulation for Estimating of Gamma Ray Attenuation of Nano - Mercuric Oxide into Nano - Bentonite Samples

A. M. Ali[1], W. A. Ghaly[2]

[1, 2]Department of Physical Sciences, College of Science, Jazan University, P. O. Box.114, Jazan 45142, Kingdom of Saudi Arabia
[2]Corresponding author's email: *wghaly[at]jazanu.edu.sa*

Abstract: ***The present work presents estimation of the gamma rays and neutrons attentions for samples of Nano - mercuric oxide (N - HgO) into Nano - Bentonite (N - Bent) based on using (100 - x% N - Bent x% N - HgO, x = 10, 20, 30, and 40 wt %). A comparison study between experimental results and simulation is demonstrated. MCNP code is used to simulate the penetration of gamma rays and neutrons through the samples. MCNP code and Phy - X/PSD software programs were also used to calculate some parameters for shielding such as effective atomic number (Zeff), mass attenuation coefficient (MAC), linear attenuation coefficient (LAC), tenth value, half value layers (TVL, HVL), mean free path (MFP) and effective electron number (Neff) of the samples. The samples under investigation are of densities ranging from 2.447 g/cm^3 to 3.647 g/cm^3. Both results of Phy - X/PSD and MCNP are compared to experimental results from papers containing the same samples under study. MCNP and Phy - X/PSD software programs show good agreement in the studied energy range. Sample 5 - Hg shows better shielding properties than the other samples.***

Keywords: Gamma ray, shielding, Nano - mercuric oxide target, Monte Carlo simulation method and Phy - X/PSD program

1. Introduction

Gamma ray and neutron sources are used widely in medical, research centers and industry such as petrochemical and refinery industries, steel factories, …. etc. Recently bulk materials doped with nanomaterials (NMs) become a topic of internets for shielding from Gamma rays (Mokhtari K. et. al., 2021 & Nikbin I. M. et. al., 2020 and Afkham Y. et. al., 2020).

Computer simulation and computational methods are used to estimate the attenuation of gamma rays (Briesmeister J. F., 2000). Moreover, Monti Carlo simulation and PhyX/PSD codes are used in many research studies to investigate gamma ray penetration through different materials (Afaneh F. et. al., 2022, Moradi F. et. al., 2019, Gurinder P. S. et. al., 2020 and Ghoza M. H., 2023).

In present work, a study is being conducted on the interaction of gamma rays and neutrons with a bulk material doped with Nano - mercuric oxide (N - HgO) into Nano - Bentonite (N - Bent) based on using (100 - x% N - Bent x% N - HgO, x = 10, 20, 30, and 40 wt %). The samples were investigated by MCNP 4C code and Phy - X/PSD program. A comparison between the simulation results and experimental results in addition to calculation using equations done by Allam E. A. et. al., 2022 is presented.

Table 1: Chemical composition by weight, thickness, density and weight fraction of elements of the prepared N - HgO/N - Bent samples (Allam E. A. et. al., 2022)

Sample name	Chemical composition (wt%)		Thickness (cm)	Density (g. cm^{-3})	Weight fraction of elements					
	HgO	$Al_2H_2Na_2O_{13}Si_4$			Hg	Al	H	Na	O	Si
1 - Hg	0	100	0.25	2.447	0	0.1278	0.0048	0.01089	0.4925	0.226
2 - Hg	10	90	0.25	2.664	0.0926	0.115	0.0043	0.098	0.4507	0.2394
3 - Hg	20	80	0.25	2.976	0.1852	0.1022	0.0038	0.0871	0.4088	0.2128
4 - Hg	30	70	0.25	3.239	0.2778	0.0895	0.0033	0.0762	0.3669	0.1862
5 - Hg	40	60	0.25	3.647	0.3705	0.0767	0.0029	0.0653	0.3251	0.1596

2. Materials and Methods

This study is intended to evaluate the radiation shielding performance of Nano - mercuric oxide (N - HgO) into Nano - Bentonite (N - Bent) samples using Phy - X/PSD program and Monte Carlo simulation MCNP 4C code. The chemical composition and physical properties of the samples has been taken from Allam E. A. et. al., 2022, and are shown in table 1. The method of calculation of different shielding parameters are given and discussed in the following sections.

2.1. A Gamma - ray shielding parameters

The performance of shielding materials against gamma photons can be performed by evaluating different parameters such as HVL, MAC and Z_{eff}. Mass attenuation coefficient MAC in (cm^2/g) is the most important parameter which describes the photon penetration in materials, which can be computed by the following relation:

$$I = I_0 e^{-\mu x} \quad (1)$$

$$MAC = \left(\frac{\mu}{\rho}\right) = \frac{ln\frac{(I_0}{I)}}{\rho x} \quad (2)$$

Where I_0 is incident beam and I is transmitted beam, x is the mass thickness and ρ is density of investigated sample. μ is linear attenuation coefficient (LAC)

HVL estimate directly the layer thickness needed to absorb the radiation by factor of ½. HVL can be calculated from (μ) as follows (Taqi A. H., et. al., 2021, Reda A. M. et. al., 2020, Tellili B., et. al., 2017, Elmahrough Y., 2015)

$$HVL = \frac{0.693}{\mu} \quad (3)$$

The electronic cross - section (σ_e) and atomic cross - section (σ_a), could be obtained by equations 4, 5 (Taqi A. H., et. al., 2021, Reda A. M. et. al., 2020, Tellili B., et. al., 2017, Elmahroug Y., 2015, Reda A. M., 2021) :

$$\sigma_a = \frac{\frac{\mu}{\rho}}{N_A \sum_i \frac{W_i}{A_i}} \quad (4)$$

$$\sigma_e = \frac{1}{N_A} \sum_i \frac{f_i A_i}{Z_i} \left(\frac{\mu}{\rho}\right)_i . \quad (5)$$

Where N_A is the Avogadro's number and w_i is fractional weight, A_i is atomic weight, f_i is fractional abundance, Z_i is atomic number, μ is linear attenuation coefficient (LAC), and $(\mu/\rho)_i$ is mass attenuation coefficient (MAC) of the i^{th} element in the composition of the shielding material.

Effective atomic number (Z_{eff}) could be evaluated by equations 6

$$Z_{eff} = \frac{\sigma_a}{\sigma_e} \quad (6)$$

2.2 MCNP simulation

MCNP 4C code can be used to simulate the penetrated flux of gamma rays through investigated Nano - mercuric oxide (N - HgO) into Nano - Bentonite (N - Bent) samples. In MCNP 4C simulation, gamma ray source is isotropic, monochromatic point source, photon mode is used, the photon importance is one inside all cells and zero in cutoff area. Flux of transmitted gamma rays is estimated using F4 tally. Figure 1 shows the geometry of the simulation. The geometry consists of source collimator, detector collimator and investigated sample with the dimension shown in figure 1. The transmitted gamma photons are calculated behind different layer thicknesses (1 - 5 cm) of each sample then the mean value is calculated. The elemental analysis of investigated samples was input to MCNP 4C code.

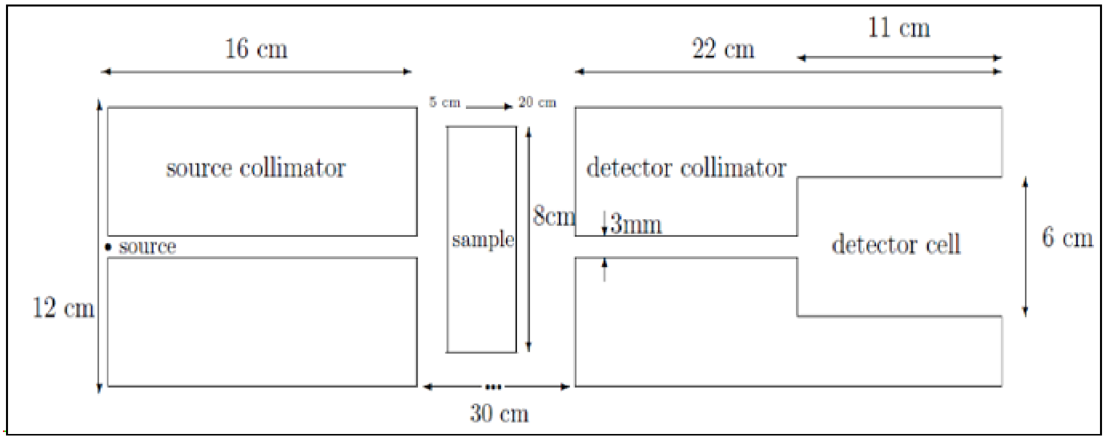

Figure 1: Geometrical design of MCNP4c simulation of penetrated gamma rays through Hg samples.

3. Results and Discussion

3.1 Mass attenuation coefficient (MAC)

The most crucial parameter to be studied and which can be used to characterize the material absorbing is Mass attenuation coefficient (MAC). For better gamma radiation protection materials, MAC should be higher (Attix. F., 1986). The obtained results of mass attenuation coefficient (cm^2/g) for the investigated samples, have been shown in figure 2.

MAC of each sample estimated by both MCNP 4C and Phy - X/PSD codes are displayed in figure 2. In addition, the calculations are comparing with the experimental results by Allam E. A. et. al., 2022. Figure 2 shows an excellent agreement between MCNP, Phy - X/PSD and the experimental results for 1 - Hg sample. For the sample 2 - Hg to 5 - Hg, the results show higher mass attenuation coefficient than the other samples and 1 - Hg samples shows the lowest value of MAC while the results of Phy - X/PSD are close to both results. From figure 2, it is clear that 4 - Hg and 5 - Hg samples have higher values of mass attenuation coefficient which means that these samples have higher shielding performance than the other samples.

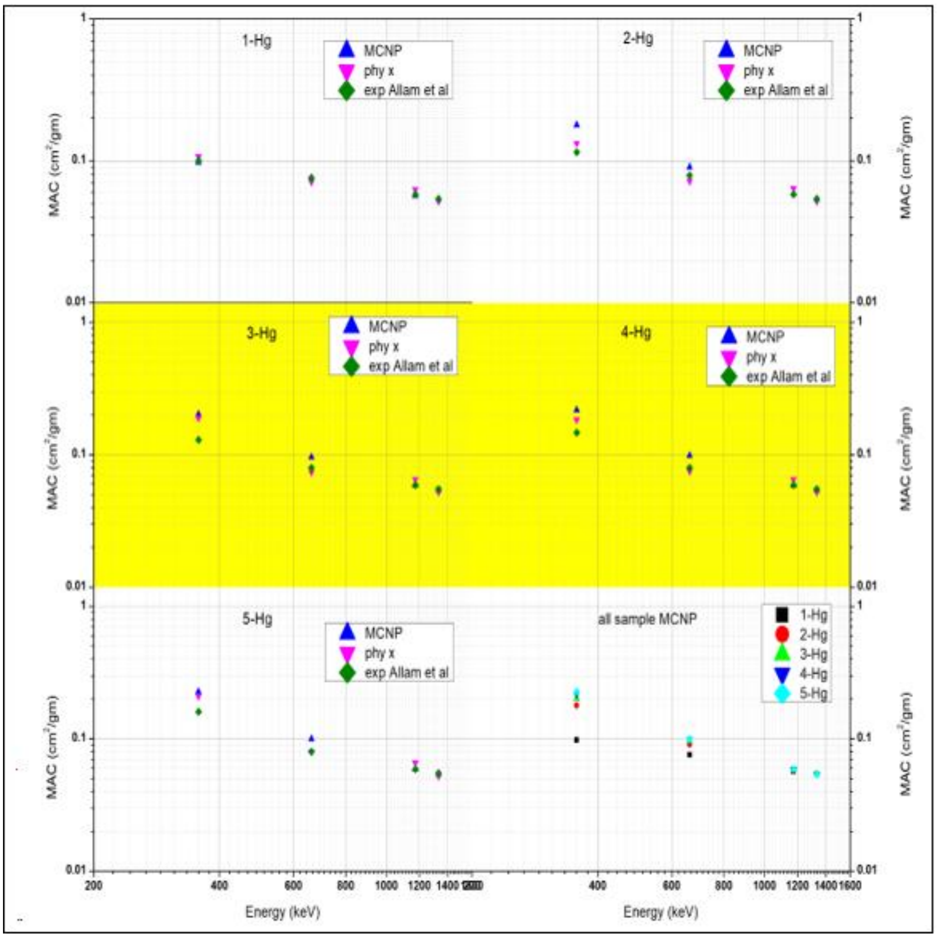

Figure 2: Variations of MAC for the investigated samples (1 - Hg to 5 - Hg) versus photon energy in KeV.

3.2 Linear attenuation coefficient (LAC)

Linear attenuation coefficient is another crucial parameter to estimate the attenuation shielding of the investigated samples against gamma - rays. The results are calculated by MCNP 4C code and Phy - X/PSD software program and compered with the experimental results by Allam E. A. et al., 2022. The variation of linear attenuation coefficient for the studied samples against photons energy was displayed in figure 3. Figure 3 shows LAC of each sample estimated by both MCNP 4C code and Phy - X/PSD software program. Figure 3 shows an excellent agreement between Phy - X/PSD and MCNP results for the sample 1 - Hg. The samples 2 - Hg to 5 - Hg shows an excellent agreement between Phy - X/PSD and MCNP results for the energy 1173 Kev while the results of other energy are deviating by values from 9% to 13%. As photon energy increases greater than 100 keV, the decreasing rate of LAC was very slow. It is due to the fact that the interaction cross section is linearly dependent on atomic number in Compton scattering region. It was observed that the difference was very small between energy range 0.2 and 2 MeV, where Compton region.

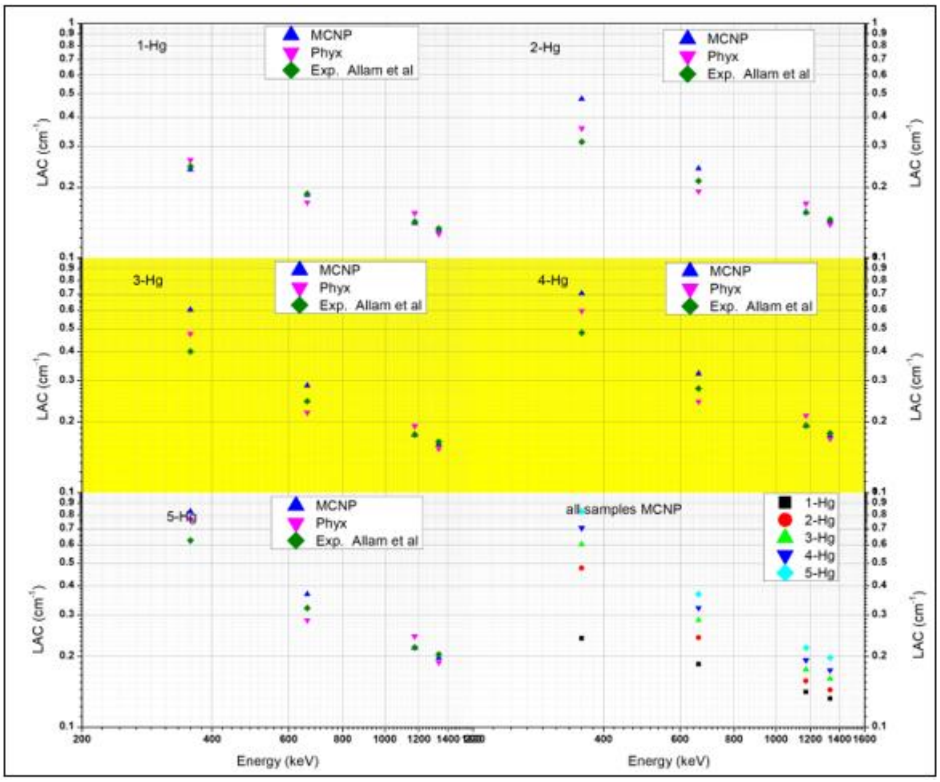

Figure 3: Variations of LAC for investigated samples (1 - Hg to 5 - Hg) versus photon energy in MeV.

3.3 Half value layer (HVL)

Half value layer determines the required thickness to absorb the half of incident intensity of gamma photons (Al - Hadeethi Y. and Sayyed M. I., 2019). Figure 4 represents the HVL for the samples under study. From figure 4, it is clear that by increasing sample density, HVL decreases. The sample 5 - Hg has highest density, so HVL is least, which shows that it has a better attenuation than the other examined samples. HVL value of 1.332 MeV photons is 5.2 cm for 1 - Hg sample and 3.4 cm for 5 - Hg sample.

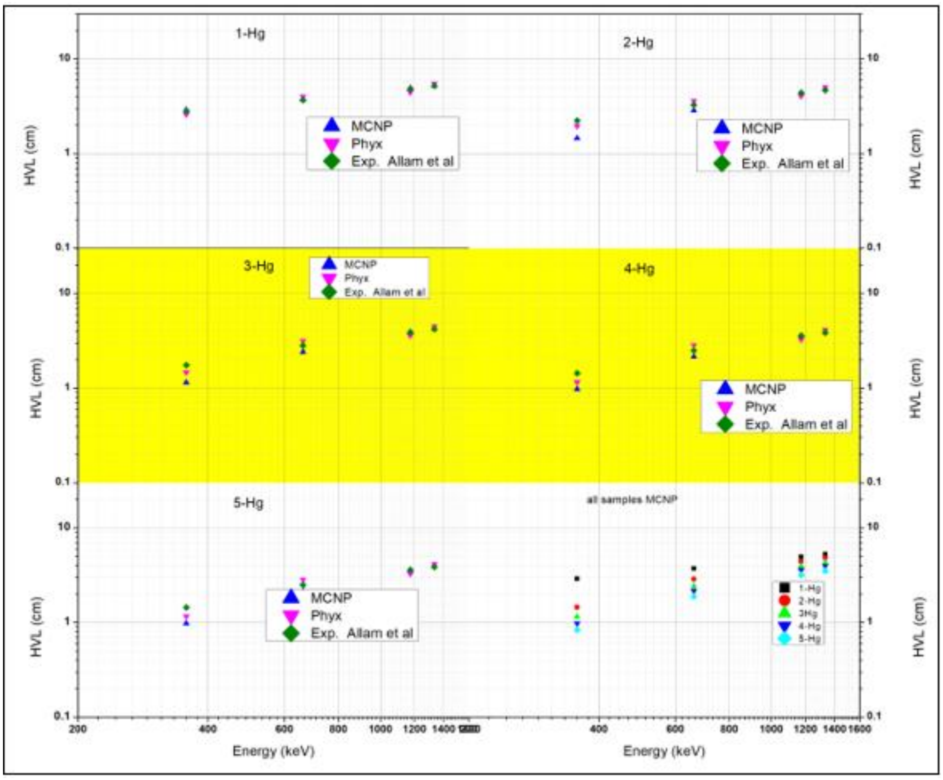

Figure 4: Variations of HVL for the investigated samples (1 - Hg to 5 - Hg) versus photon energy in keV.

Figures 4 shows an excellent agreement between Phy - X/PSD, MCNP and experimental results for the sample 1 - Hg. The samples 2 - Hg to 5 - Hg show an excellent agreement between Phy - X/PSD, MCNP and experimental results for the energy greater than 1000 keV while at the energy 662 keV there is small differences between MCNP and Phy - X/PSD results and the experimental results. Finally, at the energy 365 keV, Phy - X/PSD results are closer to the experimental results than that of MCNP.

3.4 Effective atomic number (Z_{eff})

Z_{eff} is a very useful parameter that determines the attenuation capability of studied samples. Materials of higher value of Z_{eff} have higher γ - rays shielding efficiency (Al - Hadeethi Y and Sayyed MI, 2019). The Z_{eff} calculation for the investigated samples is calculated using both MCNP 4C and Phy - X/PSD programs and compered with the experimental results by Allam E. A. et al., 2022. Figure 7 shows the relation between Z_{eff} values of the samples under investigation and photon energy. At lowest photon energy, Z_{eff} has higher values. Z_{eff} decreases rapidly in the energy range 100keV - 1MeV. After 1 MeV, the curve shows slowly increasing in the Z_{eff} values. Moreover, Z_{eff} also depends on the density of the sample. It is noted that 5 - Hg sample has largest value of Z_{eff}. These results are further in favor that examined samples can be used to have high shielding properties.

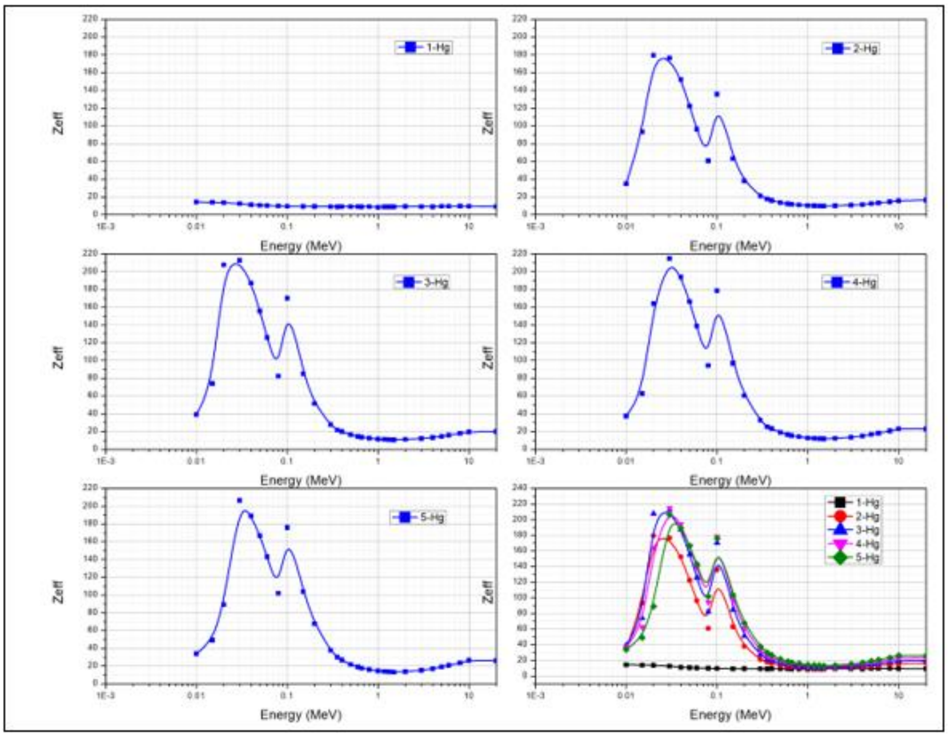

Figure 7: Variations of Z_{eff} for the investigated samples versus photon energy in keV.

3.5 Dependency of density

The mass attenuation coefficients of investigated samples for most interest energies as a function of sample density is displayed in figure 8 and table 2.

In general, the attenuation properties of materials depend on materials density but in low energy the photoelectric interaction is prevalent, so the attenuation properties are more sensitive to the atomic number (σ_{photo} α Z^5) (Das A. and Ferbel T., 2005). Mercury (Z=80) is the element of highest atomic number in the constituent of samples under investigation, so the sample of higher ratio of mercury will show more shielding efficiency.

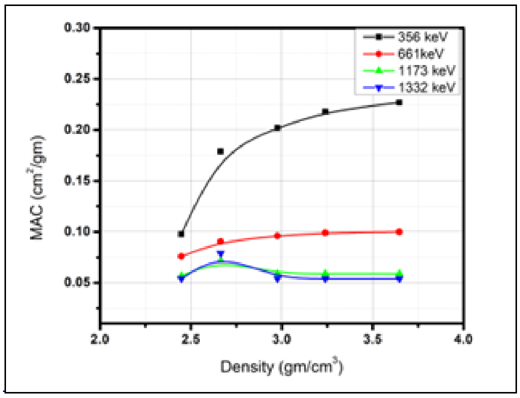

Figure 8: Variations of mass attenuation coefficient of the investigated samples versus sample density.

Table 2: MAC for different densities of samples (1 - Hg to 5 - Hg) by MCNP code.

	Mass attenuation coefficient (cm^2/gm)			
Density (g/cm^3)	356 keV	661keV	1173 keV	1332 keV
1 - Hg (2.447)	0.09767	0.07593	0.057	0.054
2 - Hg (2.664)	0.179	0.0905	0.072	0.079
3 - Hg (2.976)	0.202	0.096	0.059	0.054
4 - Hg (3.239)	0.218	0.099	0.059	0.054
5 - Hg (3.647)	0.227	0.1	0.059	0.054

4. Conclusion

In this study the photon attenuation parameters of Nano - mercuric oxide (N - HgO) into Nano - Bentonite (N - Bent) samples are calculated by Phy - X/PSD and simulation by MCNP for energies 365 keV, 661 keV, 1173 keV and 300 1332 keV. By comparing the results of Phy - X/PSD and MCNP with experimental results (Allam et. al.2022), it can be concluded that:

- The mass attenuation coefficients, linear attenuation coefficient, Half value layer, Z effective of both Phy - X/PSD and MCNP methods with the experimental results are in good agreement.
- Samples 4 - Hg and 5 - Hg have higher values of mass attenuation coefficient which means that these samples have higher shielding performance than the other samples.
- The sample 5 - Hg has highest density, so HVL is least, which shows that it has a better attenuation than the other examined samples.
- HVL values of photons of energy 1.332 MeV are in the range from 5.2 cm to 3.4 cm.
- 5 - Hg sample has largest values of Z_{eff}.
- Mercury (Z=80) is the element of highest atomic number in the constituent of samples under investigation, so the sample of higher ratio of mercury will show more shielding efficiency.
- The simulated MCNP results, which have 0.01% relative error, showed a good agreement with Phy - X/PSD values. This agreement indicates that Monte Carlo method may be used to perform more calculations on the photon attenuation characteristics of different nuclear materials.

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