



A Monte Carlo Simulation study on the Gamma Radiation Shielding Properties of Concrete with PET Plastic Composite using the PHITS Code

Myat Mon Aye¹, Thaw Tun Ko²

myatmonaye206@gmail.com, thawtunko@gmail.com

^{1,2} Department of Nuclear Engineering, Mandalay Technological University

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Abstract

The gamma radiation shielding properties of four different types of PET concretes, containing 0 %, 5 %, 10 %, and 15 % PET additives, were simulated using the PHITS code. The simulation covered photon energy levels ranging from 0.01 to 1.5 MeV and employed a NaI (Tl) scintillation detector. Parameters such as the linear attenuation coefficient (LAC), mass attenuation coefficient (MAC), half-value layer (HVL), and mean free path (MFP) were calculated to evaluate the gamma-ray attenuation for each photon energy level. The effectiveness of PET plastics as a radiation shield depends on factors like material thickness, the type of radiation, and specific application requirements. However, this research provides valuable insights into repurposing waste PET plastics to enhance the radiation-shielding properties of concrete, contributing to improved waste management practices and the development of radiation-shielding materials. The results obtained from the PHITS code align satisfactorily with both the simulation results and the theoretical XCOM data

A. Introduction

Nuclear technology has become an essential component in various sectors and industries due to its versatility and wide range of applications. These applications include material identification, agriculture, medical uses, nuclear power plants, scientific research, and industrial applications. Ensuring the safety of living organisms and systems from the harmful effects of ionizing radiation, particularly gamma rays, is of utmost importance. Gamma rays are a type of ionizing radiation that possesses sufficient energy to dislodge tightly bound electrons from atoms, resulting in the creation of ions. These ions can trigger chemical reactions within cells, potentially causing DNA damage and other detrimental effects. The development of radiation shielding has been and continues to be a significant focus in optimizing radiation protection. A commonly employed strategy for effective protection against gamma-ray and neutron radiation involves utilizing a combination of low-Z (low atomic number) and high-Z (high atomic number) elements in shielding materials. This approach capitalizes on the distinct properties of different elements to achieve better attenuation of radiation [1].

Concrete, a widely used construction material, contains a mix of various elements, including calcium, silicon, aluminum, and iron, which have medium to high atomic numbers. Its unique properties make it a popular choice for radiation shielding in numerous applications, including nuclear power plants, medical facilities, and industrial settings [2]. Also, the fact that additional materials (both heavy and light) with special shielding properties can be admixed as an additive or a partial replacement to fine and coarse aggregates makes it an attractive material. The recycling of plastic waste in concrete offers significant advantages due to its widespread usage and extended lifespan, resulting in the long-term removal of waste from the waste stream [3]. Moreover, the incorporation of post-consumer plastic waste in concrete not only provides a safe disposal method but also has the potential to enhance concrete properties such as tensile strength, chemical resistance, drying shrinkage, and creep over both short and long-term durations [4].

Gamma-ray interactions in materials are indeed distinguished by partial interactions, namely photoelectric absorption, Compton scattering, and pair production. These interactions are dependent on both the energy of the gamma-ray and the atomic number (Z) of the material. Low atomic number materials, such as polymers and plastics, are widely used in various medical applications as tissue equivalents and phantom materials. These materials serve as important tools in medical imaging and radiation therapy for simulating human tissues and organs. They are particularly useful for calibrating and verifying the accuracy of medical imaging devices and radiation therapy treatments. Polymers are also used in radiation shielding applications, serving as both primary and secondary barriers against gamma radiation in medical facilities [5].

In this particular study, the focus was on calculating the mass and linear attenuation coefficients of concrete with PET plastics composite. The ability of radiation attenuation for the selected types of samples was compared by calculating the number of gamma photons at

a specific energy range of 0.01-1.5 MeV. A NaI (Tl) scintillation detector was utilized for this purpose. Furthermore, the research evaluated the shielding effectiveness of the selected samples by examining their half-value layer, tenth-value layer, and mean free path parameters. The photon attenuation parameters were determined using the PHITS simulation code and XCOM programs.

B. Research Methods

Linear Attenuation Coefficient (LAC)

The determination of the attenuation coefficient is a crucial aspect in characterizing the diffusion and penetration of gamma rays within a specific medium [6]. Equation (1) for the attenuation coefficient quantifies the likelihood of all potential interactions between gamma rays and atomic nuclei, making it essential for addressing various issues in radiation physics and dosimetry. The determination of the attenuation coefficient is a crucial aspect in characterizing the diffusion and penetration of gamma rays within a specific medium [7]. Equation (1) for the attenuation coefficient quantifies the likelihood of all potential interactions between gamma rays and atomic nuclei, making it essential for addressing various issues in radiation physics and dosimetry. The linear attenuation coefficient μ is a crucial factor in radiation shielding as it signifies the likelihood of a photon interacting with a specific material over a given distance.

When gamma radiation passes through matter, it is primarily absorbed through interactions such as Compton scattering, photoelectric effect, and pair production. As a result, the intensity of the radiation decreases as the thickness of the absorbing material increases. The Lambert-Beer law offers the formula for intensity, which can be expressed as follows:

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

where I_0 is the beam's initial intensity, I_x is the intensity transmission to thickness x through an absorber and μ is the absorbing material's linear attenuation coefficient.

Rearranging equation (1) and applying the logarithm to both sides yield the following expression.

$$\mu = \frac{1}{x} \ln \left(\frac{I_x}{I_0} \right) \quad (2)$$

Mass Attenuation Coefficient (MAC)

The mass attenuation coefficient, represented by μ_m , is essential in studying the interaction between radiation and matter. It offers important insights into the amount of energy that is absorbed or scattered. In essence, it measures the probability of interaction between incoming photons and the material, considering the thickness of the material per unit area.

This coefficient serves as a fundamental parameter in the computation of photon penetration and energy deposition in various applications, including biological studies, shielding materials, and dosimetry. The value of μ_m , as expressed in equation (2), relies on

factors such as the energy of the incident photons, the chemical composition and bonding of the absorbing material, as well as the thickness and density ρ of the material [8]. The mass attenuation coefficient (μ_m) is derived by dividing the linear attenuation coefficient by the material density (g/cm^3), revealing the relationship between radiation and material density [9].

$$\mu_m = \frac{1}{\rho x} \ln \left(\frac{I_0}{I_x} \right) \quad (3)$$

Half-value layer (HVL)

The half-value layer (HVL) is an essential measurement that determines the thickness of a material where 50% of the incident energy has been reduced. This parameter holds great significance in comprehending the interaction between gamma rays and the material, and it is contingent upon the linear attenuation coefficient. The HVL is quantified in units of distance, specifically centimeters. Equation (4) provides a precise definition of the half-value layer for the shielding material under a given intensity [10].

$$\text{HVL} = \frac{\ln 2}{\mu} \quad (4)$$

Mean Free Path (MFP)

The mean free path is a term used to describe the average distance traveled by gamma rays in a medium before experiencing any interaction [11]. This value can be obtained by simply taking the reciprocal of the attenuation coefficient, as shown below:

$$\text{MFP} = \frac{1}{\mu} \quad (5)$$

PHITS Monte Carlo Simulation Code

PHITS (Particle and Heavy Ion Transport code System) is a Monte Carlo particle transport simulation code that has been developed by the Japan Atomic Energy Agency (JAEA) and other esteemed institutions. Its purpose is to simulate the transport of particles, including neutrons, protons, and heavy ions, and their interactions with materials and detectors. This code system plays a crucial role in numerous research fields, such as radiation shielding, radiological protection, and medical physics. By employing different nuclear reaction models and data libraries, PHITS enables the simulation of particle transport with energy [12].

PHITS, a software written in Fortran, can be compiled using Intel Fortran 11.1 or later versions, as well as G Fortran 4.7 or 4.8. It is compatible with Windows, Mac, and Linux operating systems. To enhance its performance, PHITS utilizes distributed and shared memory parallelization techniques through Message Passing Interface (MPI) protocols and open multi-processing (Open MP) directives, respectively. Furthermore, it supports hybrid parallelization by combining both MPI and Open MP. By implementing "tally" estimator

functions, PHITS provides a wide range of quantities that can be obtained through simulation, such as heat deposition, track length, and production yields. Additionally, the estimation of radioactivity's time evolution can be achieved by incorporating DCHAIN-SP, which is a component of the PHITS package [13].

XCOM calculations

XCOM, an online database developed by the National Institute of Standards and Technology (NIST), serves as a valuable resource for understanding the interaction of photons (X-rays and gamma rays) with matter in the fields of radiation shielding and protection. It includes comprehensive datasets on photon interaction cross-sections, mass attenuation coefficients, energy absorption coefficients, and other relevant data. The XCOM database provides information for a wide range of elements, compounds, and mixtures. It covers a broad energy range, typically from 1 keV to 100 GeV, and includes data for both coherent and incoherent scattering, photoelectric absorption, and pair production [14].

XCOM provides valuable information for researchers, engineers, and radiation safety experts who work in fields where understanding and controlling the interaction of photons with matter is critical for safety, precision, and effectiveness. The XCOM database can be accessed online through the NIST website or through software that integrates XCOM data, such as Monte Carlo simulation programs.

In the present investigation, the mass attenuation coefficient for the selected concrete sample in the gamma rays transport calculations is expressed in the equation:

$$\left(\frac{\mu}{\rho}\right) = \sum_i^n \omega_i \left(\frac{\mu}{\rho}\right)_i \quad (6)$$

where $(\mu/\rho)_i$ represents the mass attenuation coefficient of the i^{th} element obtained from XCOM database.

Materials

Concrete has been produced using Ordinary Portland Cement (43 grade) and the fine aggregate consisted of pure river sand, while the coarse aggregate (gravel) was derived from crushed stone with a maximum size of 20 mm. Waste PET Plastic refers to the discarded plastic water bottles that were gathered from residential areas. Once collected, the plastic bottles were cleaned and then machine-cut into small pieces, resulting in PET fragments with an average size ranging from 3 mm to 8 mm. To incorporate the plastic content into the concrete mixture, PET strips were added at varying percentages of the cement content.

Four concrete specimens were prepared. One of the mixtures was made without incorporating PET plastics, while the other mixtures included PET as an additive, with varying 5 %, 10 %, and 15 % of cement by weight. All of the concrete samples were prepared using the same water-to-cementitious ratio, with a constant value ($w/c = 0.55$). This ratio was maintained to solely examine the impact of PET addition on regular concrete. The prepared samples were labeled as C1, C2, C3, and C4, representing the different percentages

of PET inclusion in the cement pastes 0 %, 5 %, 10 %, and 15 % respectively. The chemical contents of the concrete and PET samples were measured by an X-ray fluorescence spectrometer (XRF), tabulated in Table 1.

Table 1. Elemental compositions and density values of the investigated samples

Sample code	Sample types	Density (g/cm ³)	Elemental composition (% by weight)
C1	0% PET Concrete	2.20	Ca (45.91), Si (6.47), Mg (7.93), Al (2.17), S (0.71), K (0.60), Fe (4.20)
C2	5% PET Concrete	2.23	Ca (47.19), Si (6.55), Mg (8.20), Al (1.87), S (0.74), K (0.68), Fe (3.59)
C3	10% PET Concrete	2.29	Ca (47.26), Si (6.11), Mg (8.68), Al (1.95), S (0.75), K (0.57), Fe (4.30)
C4	15% PET Concrete	2.31	Ca (47.77), Si (5.24), Mg (6.81), Al (1.78), S (0.64), K (0.47), Fe (2.82)

Gamma Shielding Properties of Polymer Plastics

The gamma shielding properties of polymer plastics depend on factors such as their density, atomic composition, and the energy of the gamma rays. Gamma rays interact with materials primarily through the photoelectric effect, Compton scattering, and pair production. Materials with low atomic numbers (Z) are more effective at attenuating gamma rays through the photoelectric effect. Polymers, with their low atomic number elements such as carbon (C), hydrogen (H), and oxygen (O), are generally good absorbers of low-energy gamma rays, typically below 1 MeV [15].

Polymers can be advantageous for certain radiation shielding applications due to their properties, including flexibility, ease of manufacturing, and low cost. However, their effectiveness as shielding materials depends on the specific requirements of the application and the energy range of the gamma rays being shielded [16].

Monte Carlo Simulation Procedures

In the present study, the Monte Carlo simulation, specifically PHITS (version 3.240) which is a multi-purpose tool for simulating particle transport phenomena developed by JAEA (Japan Atomic Energy Agency) was used to simulate the photon attenuation coefficient of concrete with different percentages of PET additives by using of the narrow beam transmission geometrical technique [17]. During the simulations, rectangular prism materials were utilized. These materials have dimensions of 10 × 10 × 2 cm in the x, y, and z coordinates, respectively. A schematic diagram of the PHITS simulation geometry is shown in Figure 1. The gamma source was defined as a disk source with a diameter of 0.5 cm by

emitting the photon along the primary axis of the cylinder. The detector selected in this simulation was a NaI crystal, with a height of 7.62 cm and a diameter of 7.62 cm in crystal.

The calculation conditions in PHITS are established through an input file. This file contains specifications for a "t-track" tally, which calculates the photon fluence within the detector cell. This calculation involves summing the track length per source and dividing it by the cell volume.

The resulting incident (ϕ_0) and transmitted (ϕ) photon fluence are then tallied and utilized in the Lambert-Beer law to determine the mass attenuation coefficients.

$$\frac{\mu}{\rho} = \frac{\ln\left(\frac{\phi_0}{\phi}\right)}{\rho d} \quad (7)$$

where μ represents the linear attenuation coefficient, ρ is the density and d is the thickness of the sample.

To increase the accuracy of the results, each simulation was done for 10^6 gamma photons with a statistical error of less than 0.1%. By analyzing the mass attenuation coefficients (MAC), we can determine important parameters such as the linear attenuation coefficients (LAC), the half-value layer (HVL) and the mean free path (MFP). Simulation results and attenuation coefficients are compared with the theoretical values obtained from the XCOM program.

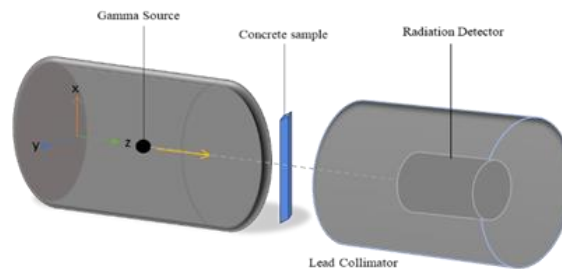


Figure 1. PHITS simulation geometry

C. Results and Discussion

Flux distribution

The penetration rate and flux spatial distribution of 0.01, 0.03, 0.05, 0.06, 0.1, 0.6, 1 and 1.5 MeV gamma photons computed by PHITS for concrete samples C1: were shown in Figure 2 respectively. The change in colors displayed the percentage difference of transmitted photons from the absorber and the distribution of flux in the field; blue and red colors represented the highest and lowest absorbance, respectively.

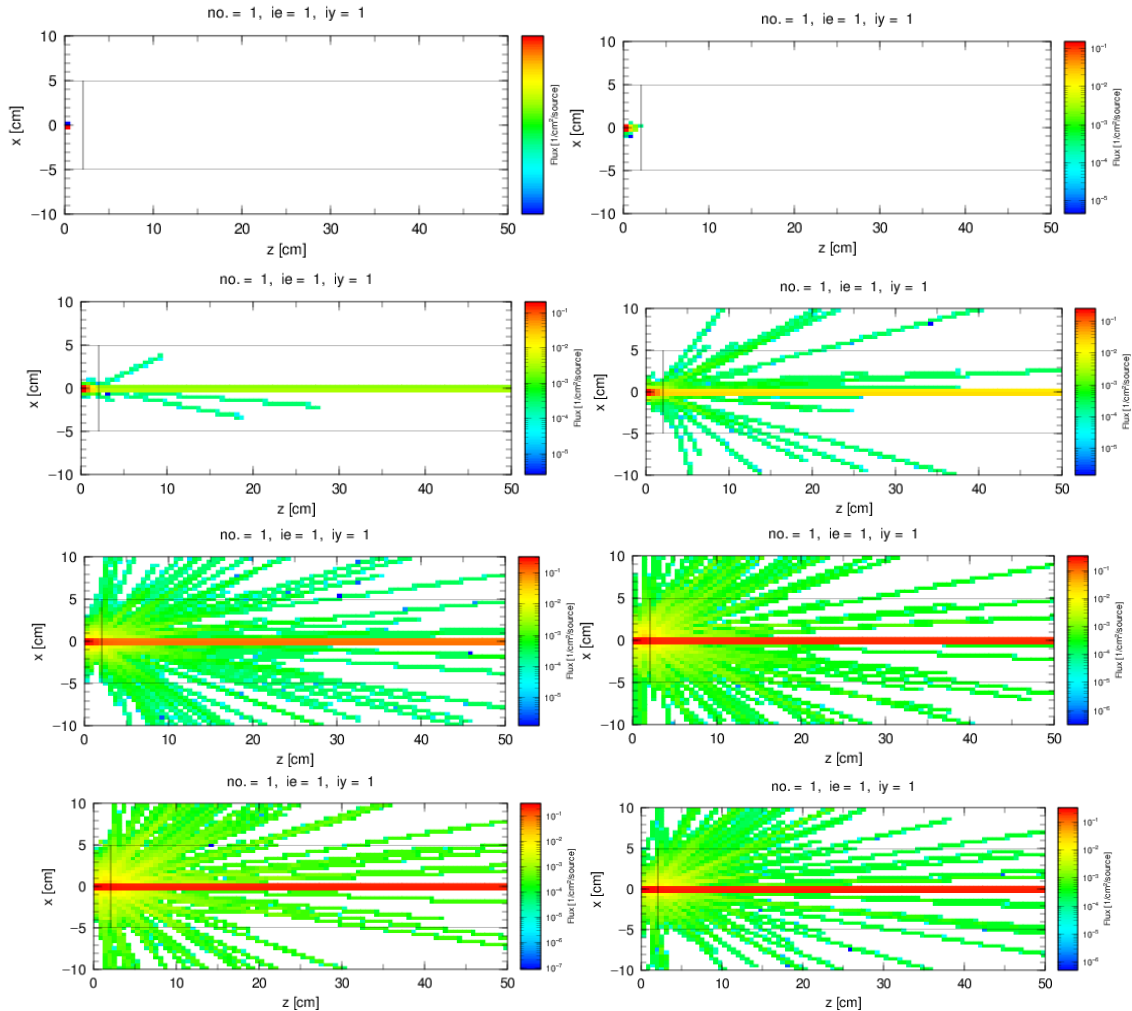


Figure 2. The penetration rate of the concrete sample computed with PHITS at the photon energies of 0.01, 0.03, 0.05, 0.06, 0.1, 0.6, 1, 1.5 MeV respectively

From Figure 2, it can be noticed that the distribution of the photon-penetration rate depends mainly on the incident photon energy and the percentage of constituent elements in the selected sample. At 0.01 to 0.03 MeV, there is no penetrating the photon by passing through the sample, although the penetrating rates are higher by increasing the photon energies from 0.05 to 1.5 MeV.

Calculation of shielding parameters

The mass attenuation coefficient of the PET concrete samples via XCOM and PHITS at different photon energies with the percentage of relative deviation can be found in Table 2. From these results, these parameters from PHITS are quite consistent with XCOM results, for which the deviation percent between both methods is less than 3%.

Table 2. Lists the mass attenuation coefficient of the samples C1, C2, C3 and C4 via XCOM and PHITS within the photon energy range of 0.01 MeV to 1.5 MeV

Energy (MeV)	C1			C2			C3			C4		
	XCOM	PHITS	Dev%	XCOM	PHITS	Dev%	XCOM	PHITS	Dev%	XCOM	PHITS	Dev%
0.01	54.910	54.710	0.37	55.260	55.240	0.04	55.500	55.498	0.04	56.350	56.348	0.18
0.015	17.510	17.490	0.11	17.640	17.620	0.11	17.720	17.718	0.01	17.970	17.968	0.50
0.02	7.7120	7.6920	0.26	7.7720	7.7700	0.03	7.8070	7.8050	0.03	7.9080	7.9060	0.03
0.03	2.4600	2.4400	0.82	2.4800	2.4780	0.08	2.4910	2.4890	0.08	2.5190	2.5170	0.08
0.04	1.1440	1.1420	0.18	1.1530	1.1510	0.17	1.1570	1.1550	0.17	1.1680	1.1660	0.17
0.05	0.6675	0.6655	0.30	0.6721	0.6701	0.30	0.6745	0.6725	0.30	0.6801	0.6781	0.29
0.06	0.4539	0.4519	0.44	0.4565	0.4545	0.44	0.4579	0.4559	0.44	0.4612	0.4592	0.44
0.08	0.2790	0.2770	0.72	0.2801	0.2781	0.72	0.2807	0.2787	0.72	0.2821	0.2801	0.71
0.1	0.2123	0.2103	0.95	0.2128	0.2108	0.95	0.2131	0.2111	0.95	0.2139	0.2119	0.94
0.3	0.1091	0.1071	1.87	0.1091	0.1071	1.87	0.1091	0.1071	1.87	0.1093	0.1073	1.86
0.4	0.0965	0.0945	2.12	0.0966	0.0946	2.11	0.0966	0.0946	2.11	0.0966	0.0946	2.11
0.6	0.0808	0.0793	1.89	0.0809	0.0794	1.89	0.0809	0.0798	1.38	0.0809	0.0796	1.63
1	0.0635	0.0625	1.60	0.0635	0.0625	1.60	0.0635	0.0624	1.76	0.0636	0.0623	2.09
1.022	0.0628	0.0618	1.62	0.0628	0.0618	1.62	0.0628	0.0617	1.78	0.0629	0.0616	2.11
1.25	0.0567	0.0557	1.80	0.0568	0.0558	1.79	0.0568	0.0557	1.98	0.0568	0.0555	2.34
1.5	0.0517	0.0507	1.97	0.0517	0.0507	1.97	0.0517	0.0506	2.17	0.0518	0.0505	2.57

Dev. % = $100 \times \frac{|\text{MAC}(\text{PHITS}) - \text{MAC}(\text{XCOM})|}{\text{MAC}(\text{PHITS})}$

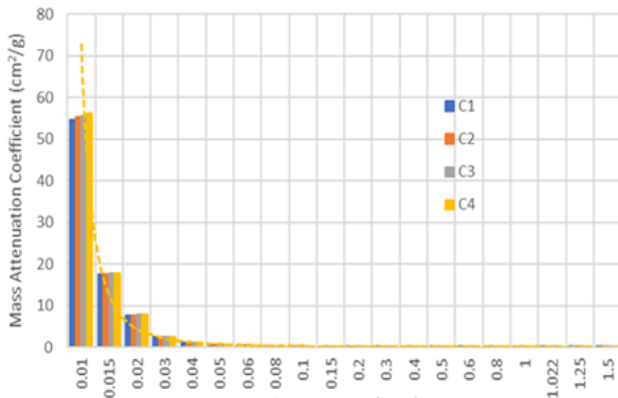


Figure 2. Mass attenuation coefficients of selected samples varies with incident photon energy

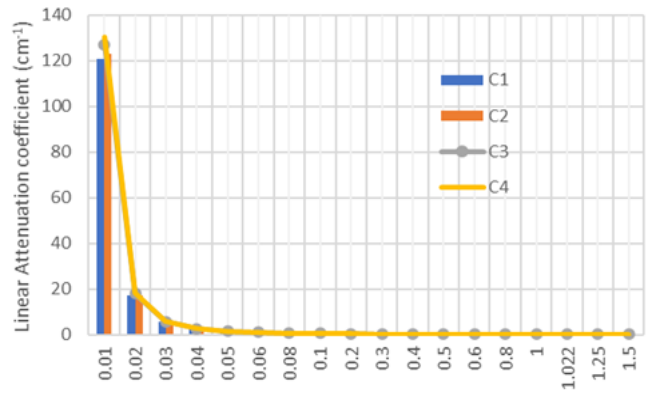


Figure 3. Linear attenuation coefficients of selected samples varies with incident photon energy

The dependence of mass attenuation coefficients (MAC or μ/ρ) and linear attenuation coefficients (LAC or μ) in the photon energy range of 0.01 to 1.5 MeV for the PET concrete samples are illustrated in Figures 2 and 3, respectively. In radiation physics, the mass

attenuation coefficient (MAC) and the linear attenuation coefficient (LAC) are two important parameters used to describe the attenuation of radiation in materials.

Figure 2 demonstrates that the MAC of all concrete samples is decreased by increasing the incident photon energy. From this figure the MAC decreased drastically with increasing photon energy in the energy region 0.01 MeV to 0.04 MeV, it decreased slightly and became constant with increasing photon energy in the energy region of 0.05 MeV to 1.5 MeV.

By seeing the tram line from Figure 3, the LAC varies with the energy of the incident photon. At 0.01 MeV, LAC is higher, although these values are smaller in the energy range of 0.05 to 1.5 MeV. The LAC sharply decreases up to 0.04 MeV and then stabilizes. At low-photon energies, the photoelectric effect dominates, while Compton interaction is effective at mid-photon energies. In the energy range of 0.05 to 1.5 MeV, MAC and LAC do not depend on the atomic number of the elements or the density of the samples. Therefore, it can be concluded that all investigated samples absorb a similar number of photons. For higher photon energies exceeding 1.022 MeV, pair production becomes dominant [18].

The attenuation coefficients are significantly influenced by the atomic number of the element and the density of the samples, particularly at low photon energies due to the photoelectric effect. Among the investigated samples, C4 exhibits the highest MAC and LAC values, while C1 has the smallest MAC and LAC values at 0.01 MeV. C4 also has the highest density, whereas C1 has the lowest density among the investigated samples. There are no significant differences in MAC and LAC of the selected samples between 0.05 and 1.5 MeV.

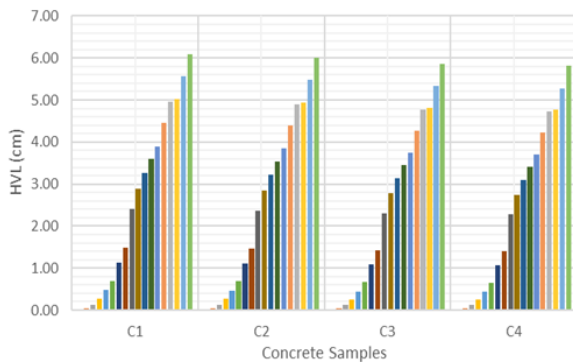


Figure 4. Variation of the half-value layer of selected concrete samples

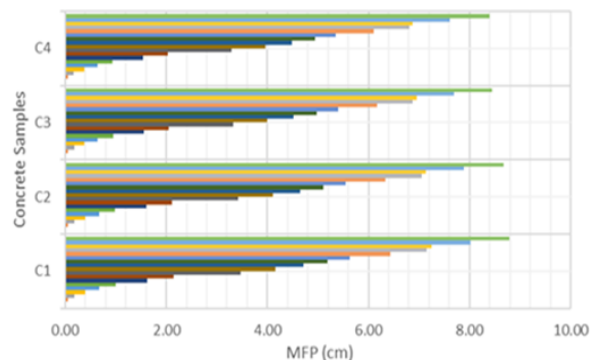


Figure 5. Variation of the mean free path of selected concrete samples

Figures. 4 and 5 illustrate the HVL and the MFP values for the investigated samples C1, C2, C3 and C4 which are dependent on the energy of the incident photon. From these Figures, the HVL and MFP of C1 exhibit the highest values, while the HVL and MFP of C4 demonstrate the lowest values among the samples under investigation. It is worth noting that HVL and MFP are inversely proportional to LAC. The order of the investigated samples in terms of HVL and MFP is $C4 < C3 < C2 < C1$. Furthermore, the HVL and MFP of the investigated samples increase as the photon energy increases. The smaller HVL and MFP of the samples indicate a higher likelihood of interaction between incident photons and matter. Consequently, smaller HVL and MFP suggest better photon absorption properties of the samples due to the reduced distance between two interactions.

D. Conclusion

The results from the simulations conducted with the PHITS code and XCOM program exhibited a high level of consistency, with a deviation of under 3%. The investigation of PET concrete samples reveals that Sample C4 demonstrates the most elevated MAC and LAC results, while Sample C1 exhibits the lowest by increasing the photon energy range of 0.01 to 1.5 MeV. By comparing the HVL and MFP values of the selected samples, it was observed that C4 had the lowest value, followed by C3, C2, and C1. These findings suggest that the studied PET concrete samples have potential applications as effective shields for radiation protection. The variations in this coefficient are influenced by the amount of PET added to the concrete mixture. The addition of PET as aggregates in the cement paste enhances its radiation shielding properties and helps to reduce the amount of non-recyclable waste in landfills. The simulation geometry technique with PHITS serves as a viable alternative method for examining the shielding parameters of various samples, particularly in scenarios where experimental findings are restricted or complex.

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