

GEANT4 Program Monte-Carlo Simulation of Ordinary Concrete's Mass Attenuation Coefficient for Gamma Rays in the Energy Range of 10 keV to 100 MeV

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Abstract: The values of mass attenuation coefficient for ordinary concrete have been simulated using the software packages GEANT4 and XCOM for gamma rays whose energies range from 10 keV to 100 MeV. Both the GEANT4 simulated data, the XCOM simulated data and the theoretical prediction were in agreement. The total mass attenuation coefficient corresponds to the sum of the mass attenuation coefficients from the individual interaction processes, namely, the photoelectric effect, the Compton effect and the electron-positron pair production. The results from both GEANT4 and XCOM showed that with the increase in gamma ray energy, there was a decrease in the photoelectric mass attenuation coefficient of ordinary concrete. The results from both GEANT4 and XCOM consistently showed a decrease in Compton mass attenuation coefficient of ordinary concrete with increase in the gamma ray energies within the above energy range. The research outcome from both simulation packages also confirmed that the electron-positron pair production mass attenuation coefficient of ordinary concrete increases with the increase in the gamma ray energy for gamma ray whose energy fall within the above range. These results were further compared to published theoretical predictions found in textbooks. The results validated the use of GEANT4 for the simulation of gamma ray attenuation in materials.

Background: The mass attenuation coefficient is a measure of a material's ability to absorb or scatter electromagnetic radiation per unit of mass. It is independent of material's density hence preferred as an attenuation parameter. It can either be experimentally obtained or theoretically through Monte-carlo methods. The GEANT4 program is one of the MonteCarlo codes in use for such studies. This research is to validate the use of GEANT4 code in studying gamma ray attenuation in materials.

Materials and Methods: The theoretical approach of Monte-carlo Simulation was employed using GEANT4 and XCOM programs to calculate the total mass attenuation coefficient for ordinary concrete. GEANT4 code and the web based XCOM code were also used to calculate the photoelectric mass attenuation coefficient, the Compton mass attenuation coefficient and the electron-positron pair production for various energies within the range of 10 keV to 100MeV.

Results: Both GEANT4 and XCOM showed that the variation of the (total)mass attenuation coefficient of ordinary concrete with gamma ray energy within the range of 10 keV to 100 MeV, from GEANT4 and the XCOM program simulated results showed good consistency except at lower gamma ray energies. The XCOM and the GEANT4 program simulated results agreed that the photoelectric effect predominates at low gamma ray photon energies, the Compton effect at intermediate gamma ray energies and the pair production at high gamma ray energies. For the gamma ray photon energy within the range of 10 keV to 100 MeV, there was an agreement from XCOM and GEANT4 programs' results that the photoelectric mass attenuation coefficient and the pair production mass attenuation coefficient of ordinary concrete decrease with increase in the photon energy. However, Compton mass attenuation coefficient decrease with the increase in gamma ray photon energy.

Conclusion: The research validated the use of GEANT4 program in the determination of attenuation parameters of different shielding materials.

Key Word: GEANT4; XCOM.

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I. Introduction

While gamma ray radiation is very important to humanity, it is also very harmful to life due to its ionizing nature. For this reason, it is important that individuals working within and around radiation facilities are under protection against these dangers. Shielding is one of the ways by which dangerous radiation exposure is

controlled and reduced. The materials of high density and high atomic number including uranium, lead, tungsten, and concrete, are most favored for use in gamma ray shielding. Whenever there is enough space, preference is always given to concrete because of its cost effectiveness and structural strength¹. In order to improve the shielding properties of concrete, a study of gamma radiation attenuation in concrete is necessary. The intensity of gamma rays is always attenuated either through scattering or absorption of the gamma ray. This is mainly through the physical interaction processes photoelectric effect, Compton effect and pair production². The attenuation parameter μ , called linear attenuation coefficient is a measure of the degree to which the intensity of an incident beam is reduced as it traverses a given medium, described by Beer-Lambert law given below,

$$I = I_0 \exp(-\mu x), \tag{1}$$

where I is the transmitted gamma ray intensity, I_0 is the incident gamma ray intensity and x the thickness of the attenuating material. Rearranging this equation gives the Linear Attenuation Coefficient^{3,4},

$$\mu = \frac{1}{x} \ln\left(\frac{I_0}{I}\right), \tag{2}$$

the mass attenuation coefficient is a measure of a material's ability to absorb or scatter electromagnetic radiation per unit of mass. Even though the linear attenuation coefficient describes the attenuation properties of a given material, it depends on the density of that material such that it is proportional to its density, ρ , which usually does not have a unique value but depends on the physical state of the material. The denser the material, the greater the probability of interaction. For materials composed of various elements the contribution of each element to the total interaction of the gamma ray follows mixture rule⁵. In this rule, the total mass attenuation coefficient of a composite is the sum of the weight proportion of each individual components as shown in equation 3. This density dependence in the linear attenuation coefficient is eliminated by expressing the attenuation properties of a given material in terms of mass attenuation coefficient (μ/ρ). For a compound or a mixture, it is given by,

$$\left(\frac{\mu}{\rho}\right) = \sum \omega_i \left(\frac{\mu}{\rho}\right)_i, \tag{3}$$

where ω_i is weight fraction and $(\mu/\rho)_i$ is mass attenuation coefficient of component i .

Depending on their energies, gamma rays interact with matter through different processes such as, Thomson scattering, nuclear photo-disintegration, nuclear resonance scattering, photoelectric effect, Compton scattering and pair-production. However, the gamma ray absorption processes is mainly dominant as photoelectric effect at low energies, Compton scattering intermediate energy range and pair production at higher energies⁶. The total cross section, a measure of the probability of any interaction to occur, can be written as the sum over the contributions from the principal gamma ray interactions as shown by equation 4 below.

$$\sigma_{Total} = \sigma_{PE} + \sigma_C + \sigma_{PP}, \tag{4}$$

where σ_{PE} , σ_C and σ_{PP} are the photoelectric effect, Compton effect and pair production cross sections, respectively.

The total mass attenuation coefficient corresponds to the sum of the mass attenuation coefficients from the individual interaction processes⁷ as in the equation below.

$$\frac{\mu}{\rho} = \frac{\mu_{PE}}{\rho} + \frac{\mu_C}{\rho} + \frac{\mu_{PP}}{\rho} = \frac{N_A}{A} \sigma_{Total}, \tag{5}$$

where ρ is the contribution of photoelectric effect, ρ is the contribution of Compton effect ρ is the contribution of pair production, N_A is Avogadro's number, A is the atomic weight, while σ_{Total} is the total atomic cross section of the material of interest.

The simulation code GEANT4⁸ and XCOM⁹ were used to study the interaction processes photoelectric effect, Compton effect and pair production involved when gamma ray gamma ray of energies between 10 keV and 100 MeV interacts with ordinary concrete material

II. Material And Methods

Both the GEANT4 and the XCOM were used to determine the mass attenuation coefficients of ordinary concrete for gamma ray whose energies range from 10 keV to 100 MeV. GEANT4 is a Monte-Carlo simulation toolkit for tracking particles through materials in a given experimental system, for which both the geometry can be designed and the physics processes can be selected by the user⁸. This simulation package is written in the programming language C++, based on the object oriented programming paradigm. It provides a

library of classes including classes for defining the geometry of the experimental system and the physics processes involved, and for generating particles. GEANT4 can be used in studies for a large set of long-lived particles, materials and elements, over a wide energy range starting, in some cases, from 250 eV and extending in others to the TeV energy range. The physics processes offered cover a comprehensive range, including electromagnetic, hadronic and optical processes¹⁰.

Generally, the GEANT4 simulation process involves defining a number of simulation aspects, namely, the geometry of the required experimental system, the physics processes involved, the response of the components of the sensitive detector, the materials to be used, the fundamental particle(s) relevant to the process, the tracking of particles as they traverse the media, the generation of primary particles for a given event, the event data generation and the acquisition of subsequent analysis of simulation data among others. The elemental composition of ordinary concrete suggested by Geant4 Collaboration¹¹ was adopted in the simulation of the mass attenuation coefficient for both of the packages. GEANT4, version 10.1 was used for this simulation. The GEANT4 simulation was based on the electromagnetic example, TestEm14 provided with the code. Ordinary concrete of 10 cm thicknesses was considered in the simulations.

The XCOM is a web based code to determine the mass attenuation coefficient for elements, mixtures and compounds⁹. In the XCOM, the mixture rule is applied to find the total and partial mass attenuation coefficients for compounds, elements and mixtures for gamma ray energies ranging from 1 keV to 1 GeV¹².

III. Result

3.1 The photoelectric effect mass attenuation coefficient

The GEANT4 and XCOM simulated contribution of the individual interactions' mass attenuation coefficient to the total mass attenuation coefficient of ordinary concrete for gamma rays within energy range from 10 keV to 100 MeV is listed in tables 1, 3 and 4 as described by equation 5.

As evident in figure 1, there was an agreement between the GEANT4 and the XCOM simulated results of the variation in photoelectric mass attenuation coefficient of ordinary concrete with gamma ray energy. In both of the simulation cases, an increase in gamma ray energy lead to a decrease in the photoelectric mass attenuation coefficient of ordinary concrete.

Table 1: GEANT4 and XCOM simulated variation in photoelectric mass attenuation coefficients of ordinary concrete with gamma ray energy.

Energy (MeV)		0.0100	0.0300	0.0600	0.0800	0.100	1.00	5.00	10.0	30.0	50.0	80.0	100
photoelectric absorption (cm ² /g)	XCOM	31.9	1.23	0.140	0.0600	0.0300	0.000	0.000	0.000	0.000	0.000	0.000	0.000
	GEANT	22.3	0.820	0.0900	0.0400	0.0200	0.000	0.000	0.000	0.000	0.000	0.000	0.000

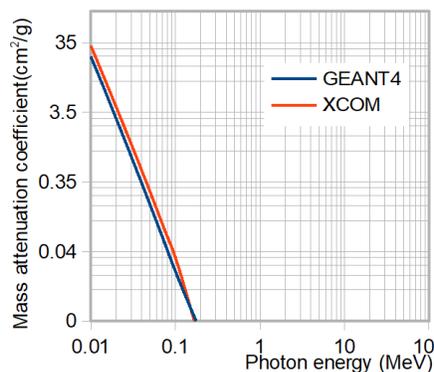


Figure 1: GEANT4 and XCOM simulated variation in photoelectric mass attenuation coefficient of ordinary concrete with gamma ray energy.

3.2 The Compton effect mass attenuation coefficient

Figure 2 shows the results of the GEANT4 and XCOM simulated variation in Compton mass attenuation coefficient of ordinary concrete with gamma ray energy. There was an agreement between the GEANT4 and XCOM calculated Compton mass attenuation coefficient. Both simulation codes shows that the Compton mass attenuation coefficient of ordinary concrete decreases with increasing gamma ray energies above 0.060 MeV.

Table 3: GEANT4 and XCOM simulated variation in Compton mass attenuation coefficient of ordinary concrete with gamma ray energy

Energy (MeV)		0.0100	0.0300	0.0600	0.0800	0.100	1.00	5.00	10.0	30.0	50.0	80.0	100
Compton scattering (cm ² /g)	XCOM	0.130	0.160	0.160	0.150	0.150	0.0600	0.0300	0.0200	0.0100	0.000	0.000	0.000
	GEANT	0.130	0.160	0.160	0.150	0.150	0.0600	0.0200	0.0200	0.0100	0.000	0.000	0.000

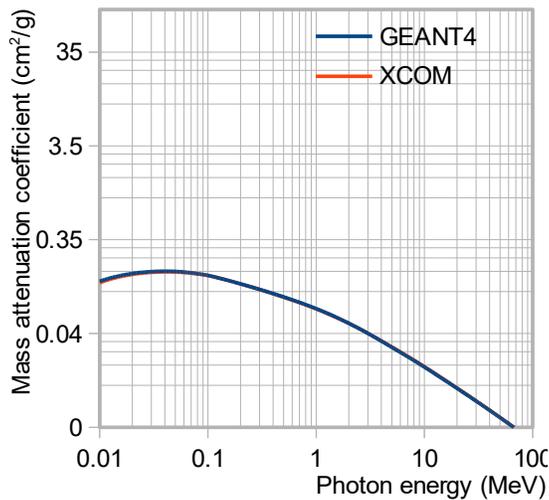


Figure 2: GEANT4 and XCOM simulated variation in Compton mass attenuation coefficient of ordinary concrete with gamma ray energy.

3.3 The pair production mass attenuation coefficient

The results on the variation of pair production mass attenuation coefficient of ordinary concrete with gamma ray energies using GEANT4 and XCOM are presented in figure 3. The pair-production mass attenuation coefficients of ordinary concrete obtained from both GEANT4 and XCOM is consistent in that it increases with photon energy for gamma rays in the energy range of 10keV to 100 MeV.

Table 4: GEANT4 and XCOM simulated variation in pair production mass attenuation coefficient of ordinary concrete with gamma ray energy

Energy (MeV)		0.0100	0.0300	0.0600	0.0800	0.100	1.00	5.00	10.0	30.0	50.0	80.0	100
pair production (cm ² /g)	XCOM	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.010	0.010	0.020	0.020	0.020
	GEANT	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.010	0.010	0.020	0.020	0.020

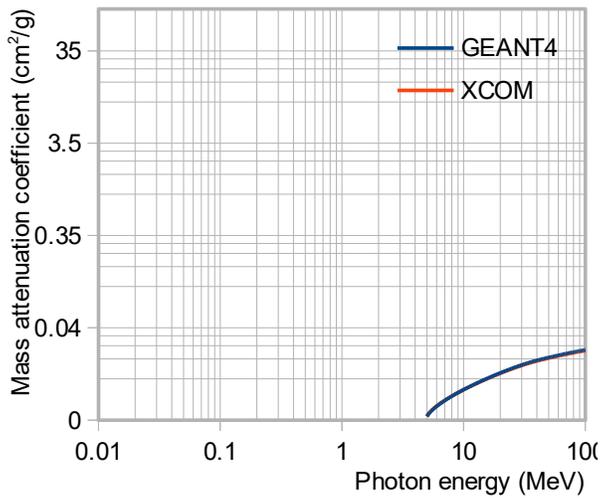


Figure 3: GEANT4 and XCOM simulated variation in pair production mass attenuation coefficient of ordinary concrete with gamma ray energy.

3.4 Total mass attenuation coefficient

The total mass attenuation coefficient of ordinary concrete for gamma ray is the sum of the individual interaction processes' mass attenuation coefficients as indicated by equation 5. This study showed that there is correspondence between GEANT4 and XCOM calculated values of total mass attenuation coefficient of ordinary concrete within the gamma ray energy range above 1 MeV as illustrated in figure 4 below. However in the gamma ray energy range below 1 MeV, a discrepancy was observed which worsened with decreasing gamma energy, where GEANT4 simulated results of total mass attenuation coefficient is systematically lower and shows a different dependence on the gamma-ray energy.

Table 5: GEANT4 and XCOM simulated variation in Total mass attenuation coefficient of ordinary concrete with gamma ray energy

Gamma Ray Energy (MeV)		0.0100	0.0300	0.0600	0.0800	0.100	1.00	5.00	10.0	30.0	50.0	80.0	100
Total attenuation (cm ² /g)	XCOM	32.0	1.39	0.300	0.210	0.170	0.0600	0.0300	0.0200	0.0200	0.0200	0.0200	0.0200
	GEANT	22.4	0.980	0.250	0.190	0.160	0.0600	0.0300	0.0200	0.0200	0.0200	0.0200	0.0200

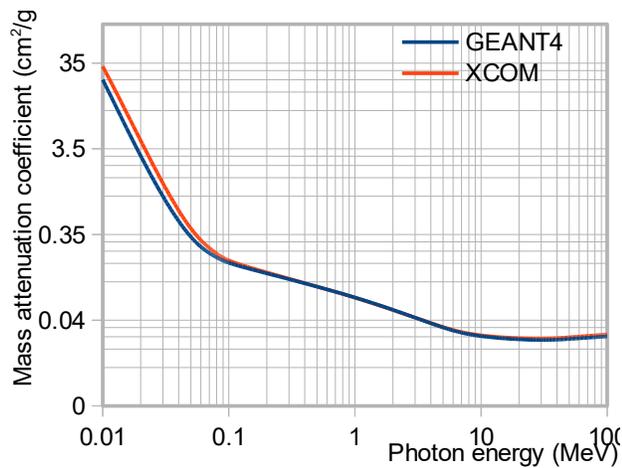


Figure 4: GEANT4 and XCOM simulated variation in Total mass attenuation coefficient of ordinary concrete with gamma ray energy.

As can be seen in the summery figures 5a and 5b, these research results confirm that the probability of a gamma ray to undergo any one of the various interaction phenomena with an ordinary concrete depends on the energy of the gamma ray. It was found that generally, the photoelectric effect predominates at low gamma ray energies, the Compton effect at intermediate gamma ray energies and pair production at high gamma ray energies. The results agreed with the indications by Podgorsak¹³ that the photoelectric effect predominates at low gamma ray energies, the Compton effect predominates at intermediate energies while the pair production predominates at high gamma ray energies.

GEANT4 SIMULATED MASS ATTENUATION COEFFICIENTS

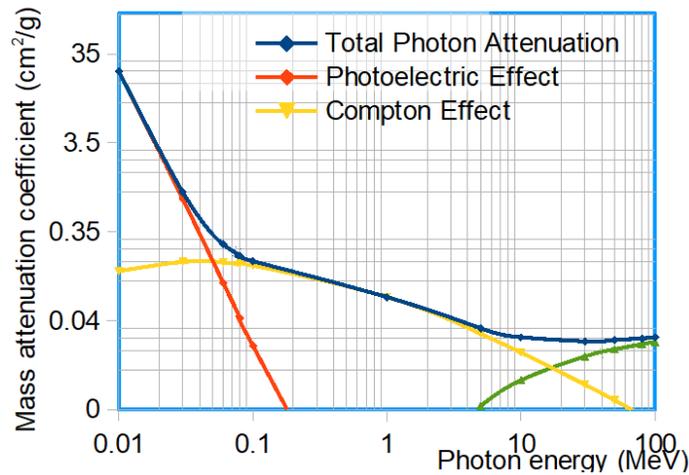


Figure 5a: GEANT4 simulated variation in the individual and total mass attenuation coefficients of ordinary concrete with gamma ray energy.

XCOM SIMULATED MASS ATTENUATION COEFFICIENTS

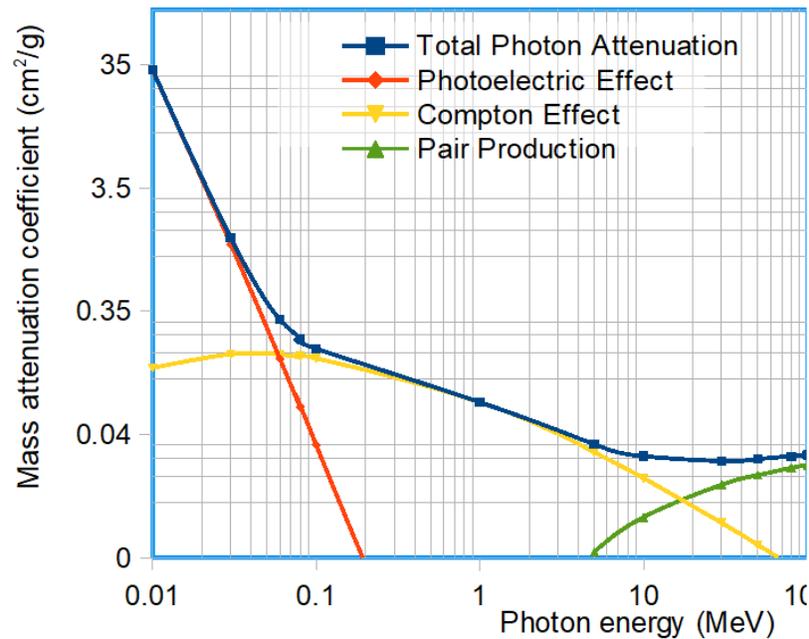


Figure 5b: XCOM simulated variation in the individual and total mass attenuation coefficients of ordinary concrete with gamma ray energy.

IV. Discussion

The observed increase in gamma ray energy led to a decrease in the photoelectric mass attenuation coefficient of ordinary concrete is consistent with both Attix's and Podgorsak's^{7,13} assertions that the photoelectric cross section(σ_{PE}) in equation 4 is gamma ray energy dependent as indicated below,

$$\sigma_{PE} \propto E_{\gamma}^{-3}, \tag{6}$$

where E_{γ} is the gamma ray energy.

However, at the lower energies, there is a slight discrepancy between the results obtained from the GEANT4 and the XCOM. This could be due to the adoption of different cross section data sources for the XCOM and the GEANT4. In the GEANT4, the low-energy photoelectric process uses the cross section data from Evaluated gamma ray Data Library "97 version"(EPDL97)¹⁴. On the other hand, the XCOM database uses data that was compiled by Scofield¹⁵ for energies below 1.5 MeV. At low energies, the uncertainty in the EPDL97 data increases with decreasing energies as shown in table 2 for solid and gaseous materials. However, for gamma ray energies above 1.5 MeV, the EPDL97 library uses the updated sub-shell cross sections of Scofield between the absorption edge energy and 1 MeV, while the total photoelectric cross sections above 1 MeV are obtained from Saloman *et al.*¹⁶. The disagreement witnessed in these results do not correspond to the systematic uncertainties presented in table 2 above, where the discrepancies are systematically lower as the energies increases. More so, for the simulated photoelectric mass attenuation coefficient, the uncertainties were above 30%, as opposed to the suggested range of 1% to 2% by Cullen *et al.*¹⁷. This could be due to the systematic uncertainties associated with the XCOM. The decreases in the Compton mass attenuation coefficient of ordinary concrete with increasing gamma ray energies above 0.060 MeV. corresponds to the indication by Attix⁷ that the Compton effect cross section(σ_C) in equation 4 is gamma ray energy dependent as shown by equation 7,

$$\sigma_C \propto E_{\gamma}^{-1}, \tag{7}$$

where E_{γ} is the gamma ray energy.

Table 2: Uncertainties of photoelectric cross sections in the EPDL97 library¹⁷.

Energy range	Solid
10 - 100 eV	1000%
100 - 500 eV	100% - 200%
0.5 – 1 keV	10% - 20%
1 – 5 keV	5%
5 – 100 keV	2%
0.1 – 10 MeV	1% - 2

Both of the simulation packages indicated that the pair production mass attenuation coefficient of ordinary concrete for gamma ray whose energies fall within the above range increases with the increase in the gamma ray energy because cross section for pair production increases with energy as was noted by both Podgorsak¹³ and Attix⁷.

V. Conclusion

In the simulation to study the variation of the mass attenuation coefficient of ordinary concrete with gamma ray energy within the range of 10 keV to 100 MeV, the GEANT4 and the XCOM simulated results show good consistency. However at lower gamma ray energies, a slight discrepancy existed between the XCOM and the GEANT4 simulated mass attenuation coefficient due to the observed difference in photoelectric mass attenuation coefficient results from the programs at low energies. This could be due to the adoption of different cross section data sources for the XCOM and GEANT4. The results from both the XCOM and the GEANT4 confirmed that the photoelectric effect predominates at low gamma ray energies (0.01 MeV to 0.1 MeV), the Compton effect at intermediate gamma ray energies (0.01 MeV to 30 MeV) and the pair production at high gamma ray energies (10 MeV to 100 MeV). On the individual processes' mass attenuation coefficient, both simulation packages indicated that the photoelectric mass attenuation coefficient of ordinary concrete decreases with increase in the gamma ray energy for gamma rays whose energies range from 10 keV to 100 MeV. The results also showed that the Compton mass attenuation coefficient of ordinary concrete decrease with the increase in the gamma ray energies within the above energy range. Finally, the results pointed out that the pair production mass attenuation coefficient of ordinary concrete for gamma rays whose energies fall within the same range increases with the increase in the gamma ray energy. The study makes it clear that both GEANT4 and XCOM can be used to study attenuation in matter.

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