Süleyman Demirel Üniversitesi
Fen Bilimleri Enstitüsü Dergisi
Cilt 28, Sayı 3, 543-550- 2024

Süleyman Demirel University
Journal of Natural and Applied Sciences
Volume 28, Issue 3, 543-550, 2024

DOI: 10.19113/sdufenbed.1549497

Theoretical Investigation of Gamma Attenuation Properties of Some Metal Oxides with GEANT4-GATE Simulation

Arzu COŞKUN *1, **Hüseyin TOPAKLI** 2

[1]Toros University, Vocational School of Health Services, 33100, Mersin, Türkiye
[2]Tarsus University, Department of Natural and Mathematical Sciences, Faculty of Engineering, 33530, Mersin, Türkiye

(Alınış / Received: 13.09.2024, Kabul / Accepted: 03.11.2024, Online Yayınlanma / Published Online: 23.12.2024)

Keywords
Gamma,
WinXCOM database,
Gate simulation,
Shielding

Abstract: This study investigated some oxide material's gamma radiation shielding properties. For this purpose, gamma radiation attenuation properties of composites formed by metal oxides MoO_2, La_2O_3, PbO, and their mixtures were examined at 50, 80, 120, 662, 1173, and 1332 keV gamma energies. Theoretical values were taken by using the GEANT-4 based GATE simulation and compared with the WinXCOM program. Using the theoretically calculated mass attenuation coefficient (MAC), linear attenuation coefficient (LAC), half-value layer (HVL), and mean free path (MFP) parameters were found. As a result of the study, it was seen that especially the MoLa(70)Pb mixture showed the best gamma shielding property with high La_2O_3 content.

Bazı Metal Oksitlerin Gama Absorpsiyon Özelliklerinin GEANT4-GATE Simülasyon ile Teorik İncelenmesi

Anahtar Kelimeler
Gamma,
WinXCOM veritabanı,
Gate simülasyon,
Zırhlama

Öz: Bu çalışmada bazı oksit materyallerin gama radyasyon zırhlama özellikleri incelenmiştir. Bu amaçla; MoO_2, La_2O_3, PbO metal oksitleri ve bunların karışımlarının oluşturduğu kompozitlerin gama radyasyonu zayıflatma özelliklerine, 50, 80, 120, 662, 1173 ve 1332 keV gama enerjilerinde bakılmıştır. Teorik değerler GEANT-4 tabanlı GATE simülasyonundan elde edilmiş ve WinXCOM programından elde edilen değerler ile karşılaştırılmıştır. Teorik olarak elde edilen kütle zayıflatma katsayısından yararlanılarak (MAC), lineer soğurma katsayısı (LAC), yarıdeğer kalınlık (HVL), ortalama serbest yol (MFP) parametreleri bulunmuştur. Çalışma sonucunda özellikle, Mo(70)LaPb karışımında yüksek La_2O_3 içeriğiyle en iyi gama zırhlama özelliği gösterdiği görülmüştür.

1. Introduction

Concurrently with technological advancements, both ionizing and non-ionizing radiation form and nuclear sources find application in several aspects of our everyday life, ranging from agriculture to food, as well as in several medical fields for diagnostic purposes. Given its extensive usage, it is imperative to quantify the potential harm it will inflict upon living beings and implement the requisite precautionary measures. Optimization should be done by providing maximum benefit with minimum dose in the definition of target material or lesion according to the purpose of use in medicine. For this purpose, the protection methods that can be taken are known as the As Low as Reasonably Achievable (ALARA) principle. Dose limits have been determined within the framework of the ALARA principle to reduce biological damage to acceptable levels [1,2]. However, especially in interventional applications (angiography) applied in medicine, the internationally permitted dose limits may be exceeded due to the prolongation of diagnosis or treatment time. The dose received by radiology workers, in particular, is increasing [3]. Protecting against radiation requires careful consideration of the three essential factors: distance, time, and shielding. Shielding is employed to limit ionizing radiation in circumstances where distance and time cannot be avoided. Concrete and lead are employed as the primary materials for shielding against radiation.

* *Corresponding author: arzu.coskun@toros.edu.tr*

Nevertheless, because of the harmful impacts of the shielding materials and the challenges of transportation, extensive research is now being conducted in the scientific community on substitute materials. Therefore, the International Atomic Energy Agency (IAEA) and World Health Organization (WHO) highly promote the development of advanced protective materials that will supplant conventional shielding materials. Especially recently, homogeneous and transparent glass materials, believed to be more widely used, are being studied. While many studies focus on glass materials for gamma-ray protection, pellets from composite materials are also used [4,5]. Li_2O-B_2O_3 glasses are traditional glass systems created widely [6,7]. In addition, with its ease of use and availability, new composite shielding materials such as polyurethane-containing shielding epoxy resin [8], high-density barite ore to shield *X*- and γ-rays, B-containing colemanite ore to stop neutron particles, and a mixture of epoxy and PbO_2 powder are available. It is intended to be produced [9]. Additionally, La_2O_3-doped borate-based glasses strengthen the recording medium for nonlinear optical devices, laser hosts, and optoelectronic memory in optical fiber cores. There are extensive studies on this type of glass [10-13]. Dong [13] investigated the mass attenuation coefficients of sources containing element B in China in the energy range of 0.001-20 MeV with WinXCOM and GEANT-4 programs [14]. Many studies compare MCNP-X and WinXCOM data to determine the properties of radiation-shielding materials. However, there are a limited number of studies investigating the properties of protective materials using the GEANT-4 based GEANT-4 application for Tomographic Emission (GATE) simulation. GATE Simulation is a freely available software that conducts Monte Carlo simulations. It is continuously enhanced by users from around the world for applications in nuclear physics, radiology, and radiation medical fields. Other software, the National Institute of Standards (NIST) WinXCOM data, contains radiation attenuation data for commonly used protective materials [15,16]. Mass attenuation coefficients can be calculated by writing the ratios and compound formulas of compounds and mixtures in the program [17]. The search for new materials as an alternative to Pb and Pb-containing materials commonly used in gamma radiation shielding continues rapidly. In the current study, oxide compounds were added to the PbO compound at different rates for this purpose.
This study investigated the gamma radiation attenuation properties of PbO, MoO_2, and La_2O_3. Firstly, the μ_m values determined by the GATE simulation code in the photon energy range of 50-1332 keV were compared theoretically with the WinXCOM Software program. MFP, HVL, and linear attenuation coefficients were also calculated using μ_m values.

2. Material and Method

To assess the radiation attenuation of gamma photons, one can analyze the mass attenuation coefficient, linear attenuation coefficient, half-value layer, tenth layer, and mean free path parameters of the materials to ascertain their shielding characteristics. The coefficient of linear attenuation is dependent on the density of the medium. More precisely, it illustrates the decrease in the number of photons per unit spatial separation from the radiation beam that passes through the material. A material's atomic number and physical density directly proportionally increase the extent of linear attenuation. Placement of an absorber between the radioactive source and the detector results in an exponential decrease in the released photons as they pass through the glass, following the Beer-Lambert equation. [18]:

$$I_x = I_0\,(e - \Gamma_x)(e - \sigma_x)(e - \kappa_x) = I_0\, e - \mu_x \qquad (1)$$

In this equality, I_x= The number of photons passing through the material, I_0= The quantity of photons reaching the material is directly proportional to the probability coefficients of the photoelectric effect, Compton scattering, pair formation, and total linearity attenuation of the material. Measurements of HVL, TVL, and MFP are calculated to evaluate the attenuation properties of gamma radiation. Half-value layer (HVL) is the minimum material thickness needed to reduce the radiation reaching the target by half. An increase in the thickness of the material produced results in a proportional decrease in the intensity of the incident photon beam. The reduction mentioned holds significant importance in the field of radiation protection. The determination of the HVL and TVL parameters is crucial in order to ascertain the shielding characteristics of materials. HVL is the material thickness that adequately decreases the initial intensity of incoming radiation by 50% by interaction with the material. The subsequent equations represent TVL values, which are defined as the material depth that decreases the intensity of incoming radiation to one-tenth magnitude.

$$X_{(1/2)} = HVL = ln2/(\mu) \qquad (2)$$

The mean free path is the average distance that incoming radiation travels between two interactions of a photon as it passes through a material, subject to the basic interactions it will undergo within the material.

$$MFP = 1/\mu \qquad (3)$$

The table below presents the density values based on the materials and mixture ratios employed in the investigation.

Table 1. Calculation of density values based on the materials and mixing ratios.

%Mole ratios

Chemical	*MoO_2*	*La_2O_3*	*PbO_2*	*density(g/cm^3)*
MoO_2	100	0	0	6,47
La_2O_3	0	100	0	6,51
PbO_2	0	0	100	9,38
MoLa	50	50	0	6,49
MoPb	50	0	50	7,92
LaPb	0	50	50	7,94
Mo(50)LaPb	50	25	25	7,21
MoLa(50)Pb	25	50	25	7,22
MoLa(80)Pb	10	80	10	6,89
Mo(80)LaPb	80	10	10	6,77
MoLa(70)Pb	20	70	10	6,79
Mo(70)LaPb	70	20	10	6,77

One of the theoretical methods used in our study, the WinXCOM program, is open access and provides mass attenuation coefficients, which are radiation attenuation parameters in the energy range of 1 keV to 100 GeV, in all matter interactions. When the mixture's formula information and energy values, compound, and elements are entered with this software program, the photoelectric effect, Rayleigh and Compton scattering, electron pair production, nuclear pair production cross sections, and mass attenuation coefficients can be calculated. In another theoretical study, the GATE detector properties of the NaI(Tl) detector were determined using the GEANT-4 based GATE simulation program. Radiation attenuation properties were investigated by placing shielding materials before the detector. GATE –WinXCOM comparison graphs regarding the radiation attenuation of each material are given below. Figure 1 shows the detector, source and material system prepared in GATE simulation.

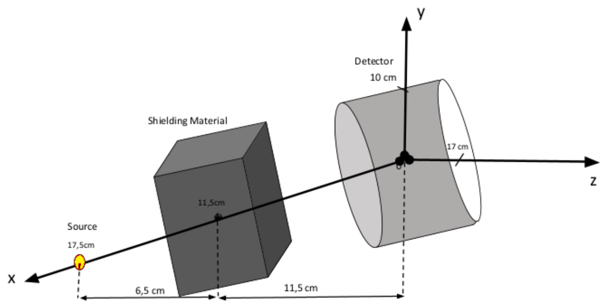
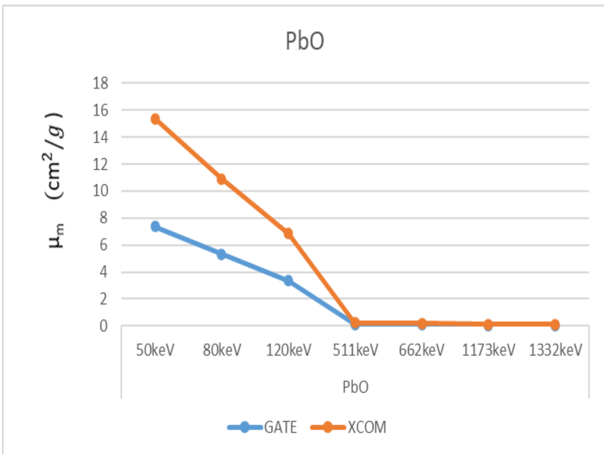


Figure 1. GEANT-4 based GATE simulation display

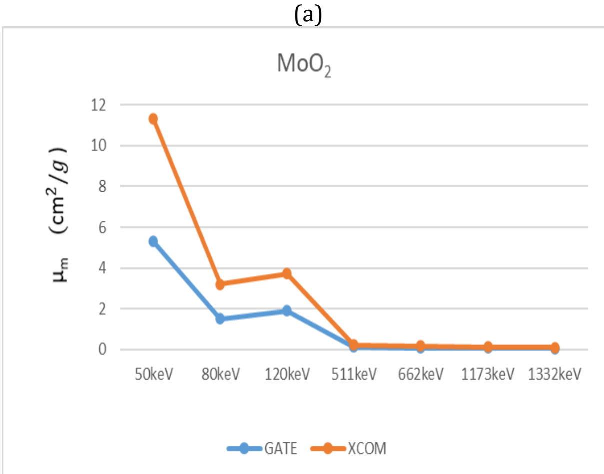
With the prepared GATE simulation setup, the NaI detector detected the mass attenuation coefficient of the shielding material placed in front of the point gamma source.
In the study by Coşkun et al., the gamma radiation shielding property of PbO compound with MoO_2 doping at 662, 1173, and 1332 keV energies was calculated with GATE simulation and XCOM (19). In the study by Tekin et al., they synthesized (65-x)B_2O_3 + 20Bi_2O_3 + 15Na_2O + xMoO_3 : x = 0, 1.5, 3, 4.5, 6 and 7.5 wt% and examined it with the program MCNPX simulation code of the composite and XCOM(20). In the study conducted by Alzahrani et. al., they investigated the optical and characteristic properties of La_2O_3–Fe_2O_3–Bi_2O_3 nanopowders as well as their gamma radiation attenuation properties with La_2O_3 additive using the XCOM program (21).

3. Results

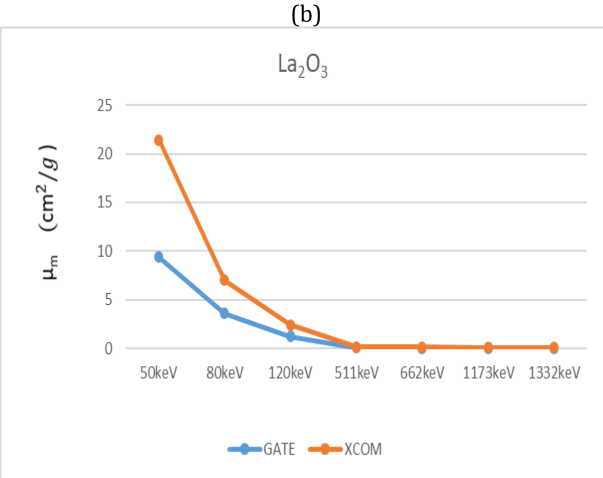
Graphs 2-15 give the same result for different compounds.



(a)

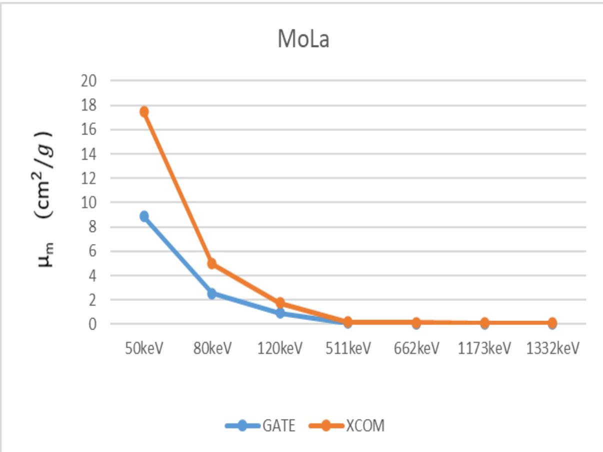


(b)

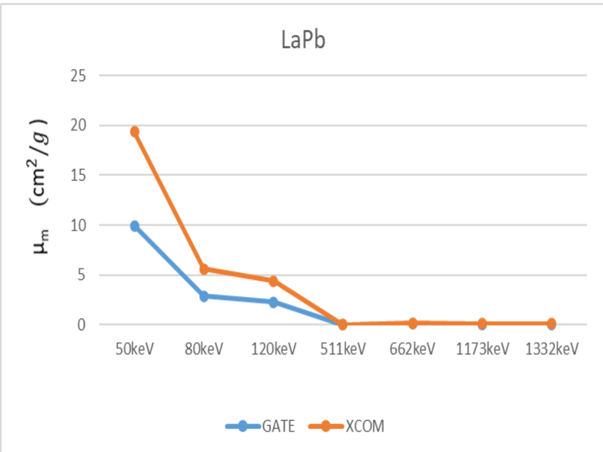


(c)

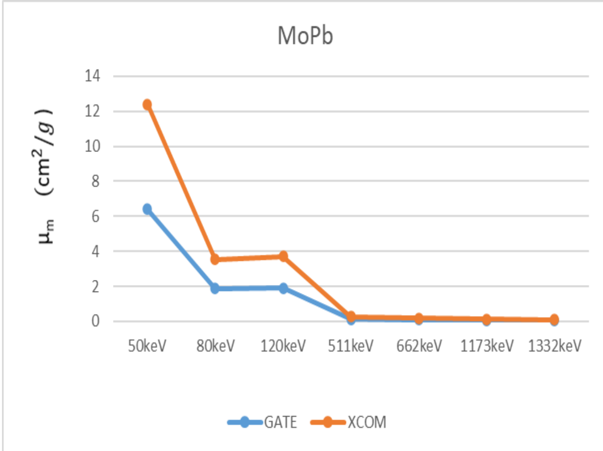
Graph 2. Mass attenuation coefficient of PbO , MoO_2 , La_2O_3 (a)-(c)



(a)

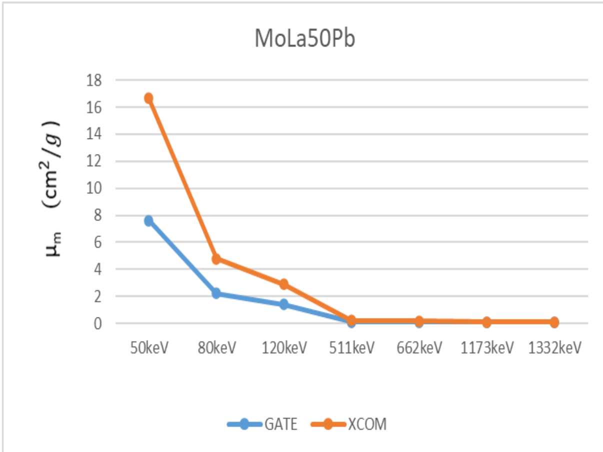


(b)

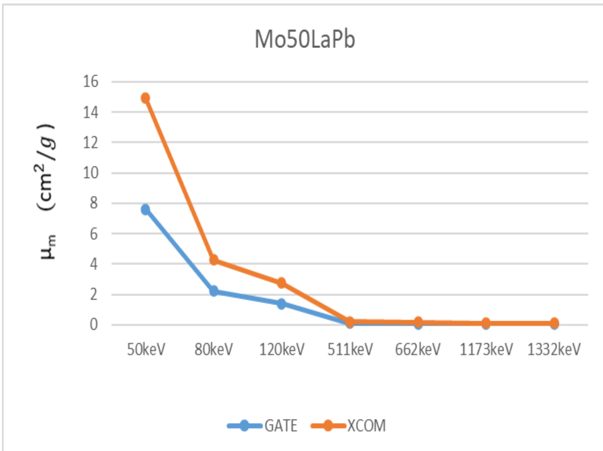


(c)

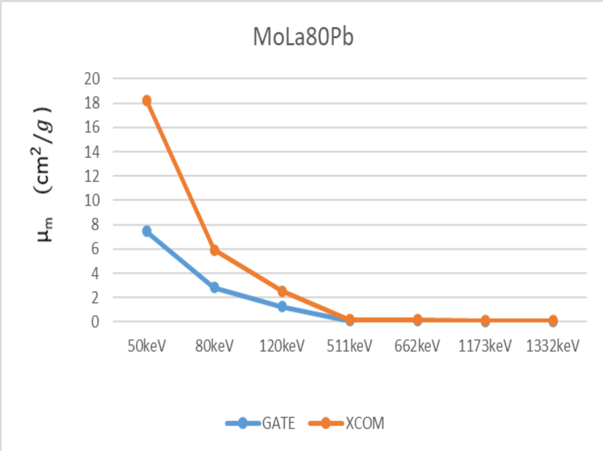
Graph 3. Mass attenuation coefficient obtained in %50 binary mixtures of compounds (a)-(c)



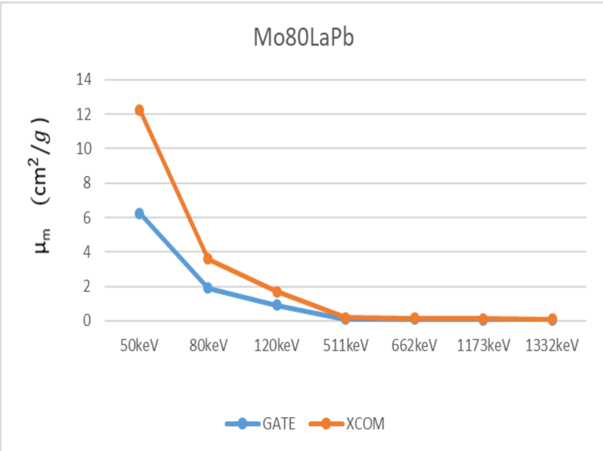
Graph 4. Mass attenuation coefficient of 20% MoO_2 and 50% La_2O_3 with constant %30 PbO



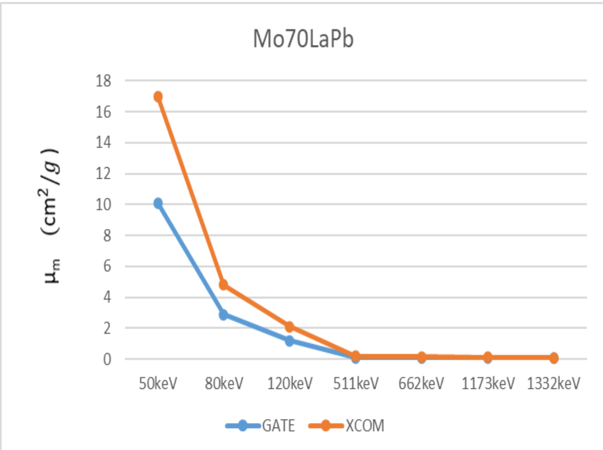
Graph 5. Mass attenuation coefficient of 50% MoO_2 and 20% La_2O_3 with constant %10 PbO



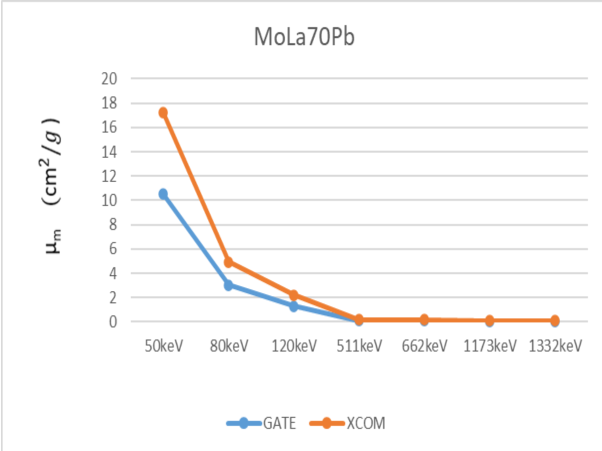
Graph 6. Mass attenuation coefficient of 10% MoO_2 and 80% La_2O_3 with constant %10 PbO



Graph 7. Mass attenuation coefficient of 80% MoO_2 and 10% La_2O_3 with constant %10 PbO

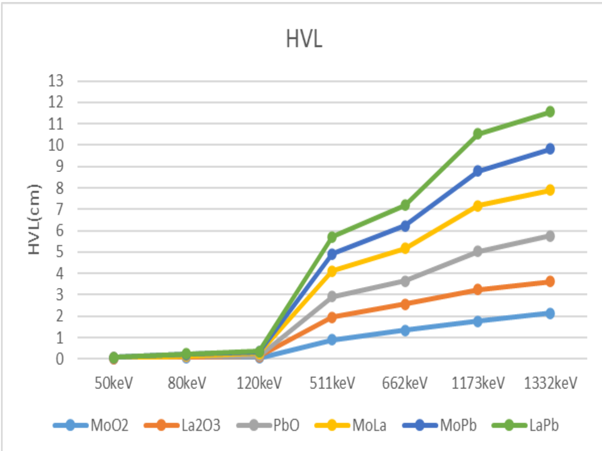


Graph 8. Mass attenuation coefficient of 70% MoO_2 and 20% La_2O_3 with constant %10 PbO

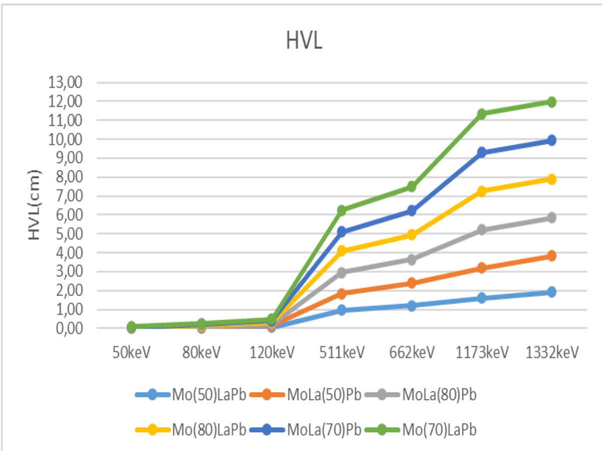


Graph 9. Mass attenuation coefficient of 20% MoO_2 and 70% La_2O_3 with constant %10 PbO

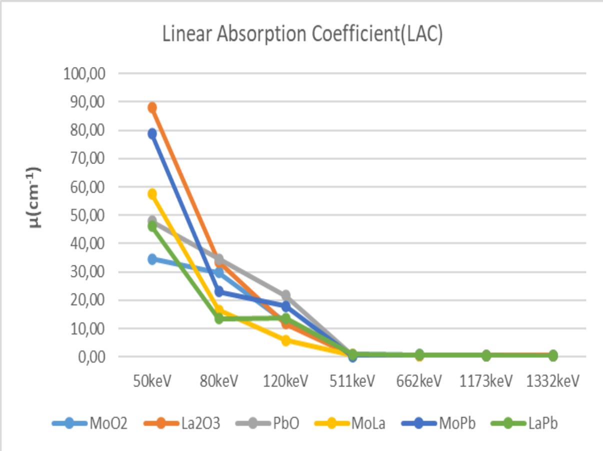
Linear attenuation coefficient, half-value layer, and mean free path data were derived from theoretical calculations of mass attenuation coefficients.



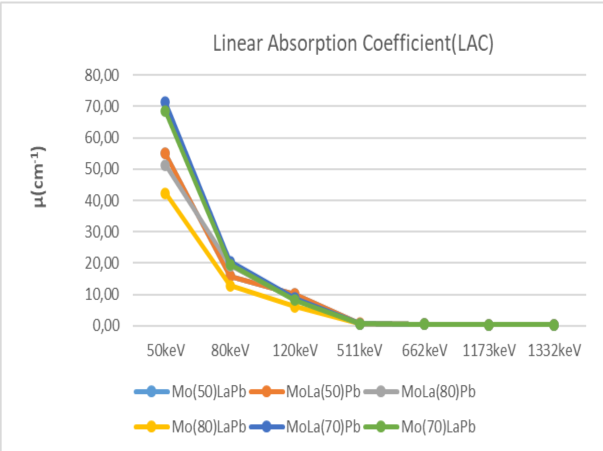
Graph 10. Half-value layer coefficient of single and binary mixtures



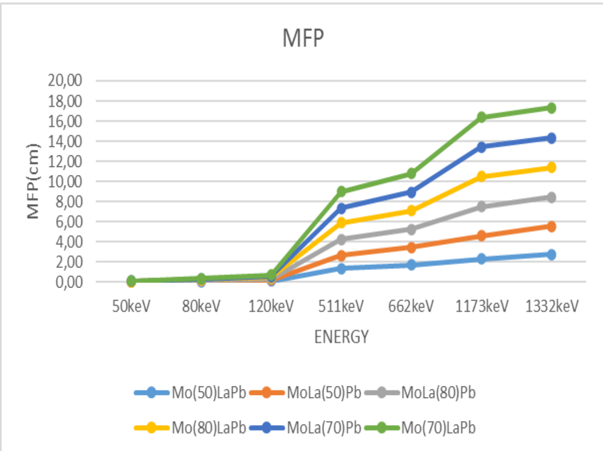
Graph 11. Half-value layer change of mixtures obtained as triple mixtures



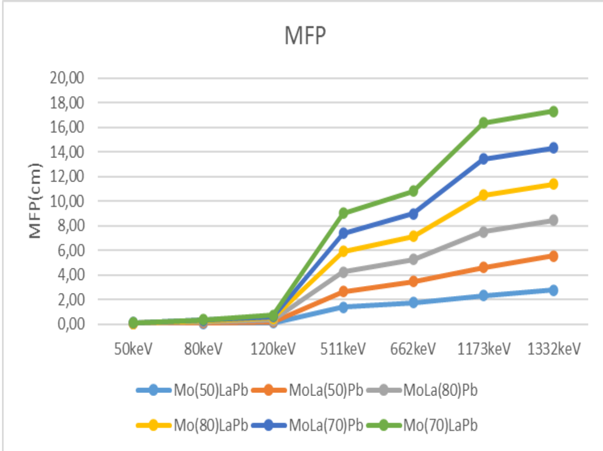
Graph 12. Linear attenuation coefficient change of single and binary mixtures



Graph 13. Linear attenuation coefficient changes of ternary mixtures



Graph 14. Mean free path change of single and binary mixtures



Graph 15. Mean free path change of ternary mixtures

4. Discussion and Conclusion

The present work aimed to examine the radiation attenuation characteristics of three particular compounds, namely PbO, MoO_2, and La_2O_3. We theoretically compared the μ_m values obtained by the GATE program within the photon energy range of 50-1332 keV with those obtained by the WinXCOM software program. In addition, the MFP, HVL, and linear attenuation coefficients were computed base on the μ_m values. It can be observed in all graphs that increasing the La_2O_3 contribution in the mixtures obtained positively affects the gamma shielding parameters. In addition, increasing the contribution as La_2O_3 increased the mass attenuation coefficient, especially in the mix named MoLa80Pb with 80% La_2O_3 contribution. When the data obtained with La_2O_3 is compared to PbO, it is seen that it has a much better attenuation value than PbO.

Both simulation and energy ranges from 356 keV to 662 keV result in a drop in the theoretical μ_m values. In the composite materials reported, the values of μ_m exhibit a significant drop as the photon energy increases. The reason for this is that the interaction between the analyzed materials and gamma radiation results in photoelectric attenuation phenomenon. Within the energy range of 1173 keV to 1332 keV, the μ_m values exhibit a modest reduction as the photon energy increases. The observed behavior can be ascribed to the compositional scattering process (CS) reaction. The shielding exhibits the highest protection capacity when the HVL, TVL, and MFP values are smaller.

Mass attenuation coefficients are given in Graph 2a-c. At a frequency of 50 keV, the PbO (Lead(II) Oxide) concentration decreases rapidly with increasing energy from GATE: 7.39 cm²/g, WinXCOM: 7.99 cm²/g to 1332 keV: GATE: 0.05 cm²/g, WinXCOM: 0.06 cm²/g. In molybdenum dioxide (MoO_2), the energy levels decrease from 50 keV: GATE: 5.3 cm²/g, WinXCOM: 6 cm²/g to 1332 keV: GATE: 0.05 cm²/g, WinXCOM: 0.05 cm²/g. The GATE/WinXCOM values for Lanthanum Oxide (La_2O_3) are 9.38 cm²/g and 12.05 cm²/g at 50 keV, respectively. The GATE/WinXCOM values at 1332 keV are 0.05 cm²/g and 0.05 cm²/g, respectively. According to the obtained results, as seen in the graphs, at low energies, close values are observed in the two simulations, while with the increase in energy, the mass attenuation coefficient (MAC) is obtained at close values due to Compton scattering. When we look at Graphs 3a-c, the mass attenuation coefficients of the binary compounds are seen. The mass attenuation coefficients of MoLa, LaPb, MoPb mixtures at 50 keV are obtained as 8.86, 9.91, 6.39 cm^2/g, respectively. After 511 keV, these values decrease to 0.05 cm^2/g. When we look at the 4th-9th graphs where the mass attenuation values of the ternary mixtures are given, it is seen that the highest mass attenuation coefficients of the MoLa50Pb, Mo50LaPb, MoLa80Pb, Mo80LaPb, MoLa70Pb, Mo70LaPb compounds are at 50 keV and are calculated as 7.62, 7.62, 7.44, 6.25, 10.5, 10.1 cm^2/g, respectively. When the graphs are examined; the highest mass attenuation coefficient on average in both simulations belongs to the MoLa(70)Pb mixture and is calculated as 9.6 cm^2/g. The linear attenuation coefficient (LAC) values are calculated by substituting the mass attenuation coefficient and density values in equation (2.1). GEANT-4 GATE simulation values were used in the calculation. Graph 12 shows the LAC results of the single and binary mixture structures. Accordingly, at 50 keV, MoO_2 gives 34.50 cm^{-1}, La_2O_3 87.98 cm^{-1} and PbO 47.81 cm^{-1}. With the increase in energy, these values become 0.33 cm^{-1}, 0.47 cm^{-1} and 0.32 cm^{-1}, respectively. In binary mixtures, especially the LaPb compound gives the highest value with 0.87 cm^{-1} at 511 keV. MoPb shows high attenuation properties at low energies. When the data obtained by mixing the compounds in Graph 13 in different ratios are examined, the highest linear attenuation coefficient value belongs to the MoLa(70)Pb mixture, and is 0.34 cm^{-1} at 1332 keV and 71.30 cm^{-1} at 50 keV. As in mass attenuation coefficients, linear attenuation coefficient decreases with increasing energy depending on interaction mechanisms with matter. A high linear attenuation coefficient indicates that radiation shielding property is high. HVL values were obtained using equation (2.2). The highest value was observed in PbO compound with 2.41 cm. HVL value increases with increasing energy. HVL value of the compound at 80 keV was calculated as 0.01 cm. Graphs 10-11 show HVL values. According to the obtained data, the highest HVL value belongs to MoLa compound, which is a binary mixture. A high HVL value indicates that radiation attenuation property decreases. Mean free path (MFP) value was calculated by replacing LAC value according to equation (2.3). The obtained results are given in graphs 14 and 15. According to the results, MFP value increases with increasing energy as in half-value thickness. It is seen in graphs 10, 11, 14 and 15 that MFP and HVL values are low where the mass attenuation coefficient is high. Accordingly, As a result, due to the high attenuation ability of composite materials against gamma radiation, shielding materials. It is also concluded that PbO is an effective shielding material at high energy levels. In addition, MoLa70Pb mixture offers the best gamma shielding properties with high La_2O_3 content. These results can be optimized for radiation protection and medical imaging and provide important information for the development of composite materials.

References

[1] Eskalen, H., Kavun , Y., Kerli S., Eken, S. 2020. An investigation of radiation shielding properties of boron-doped ZnO thin films. Optik Mater (Amst) 105 109871.

[2] Issa S., AMA, M., Hanafy , TA., Dong, M., Xue, X. 2019. Comparison study of photon attenuation characteristics of Polyvinyl alcohol (PVA) doped with Pb $(NO_3)_2$ by MCNP5 code, XCOM, and experimental results. Progress in Nuclear Energy 111.15–23.

[3] Zuguchi, M., Chida, K., Taura, M., Inaba, Y. 2008. Usefulness of non-lead aprons in radiation protection for physicians performing interventional procedures, Radiation Protection Dosimetry 131.531-534.

[4] Issa, S., Hamdalla, TA., Darwish , AAA. 2017. Effect of $ErCl_3$ in gamma and neutron parameters for different concentrations of $ErCl_3$-SiO_2 (EDFA) for signal protection from nuclear radiation. Journal Alloys Compound 698 234–40.

[5] Abouhaswa , A. S., Perişanoğlu, U., Tekin , H. O., Kavaz, E., Henaish, A. M. A. 2020. Nuclear shielding properties of B_2O_3–Pb_3O_4–ZnO glasses: Multiple impacts of Er_2O_3 additive. Ceramic International 46 27849–59.

[6] Feller, S.A., Dell , W. J., Bray P. J. 1982. 10B NMR studies of lithium borate glasses. Journal of Non-Crystalline Solids 51 21–30.

[7] Kodama, M., Matsushita, T., Kojima, S. 1995. Velocity of sound and elastic properties of $Li_2Ob_2O_3$ glasses. Japanese Journal of Applied Physics 34.2570–4.

[8] Mkhaiber, A. F., Dheyaa, A. 2018. Experimental study of some shielding parameters for composite shields. In *Journal of Physics: Conference Series* (Vol. 1003, No. 1, p. 012109). IOP Publishing.

[9] Demir, F. 2009. Determination of radiation absorbance of heavy concretes with boron and barite aggregates for neutron particles, x, and ɣ rays. Atatürk University, Institute of Science, PhD Thesis, Erzurum.

[10] Chakraborty, I. N., Shelby, J. E., Condrate, R. A. 1984. Properties and structure of lanthanum borate glasses. Journal American Ceramic Society 67. 782–785.

[11] Chakraborty, I. N., Day, D. E. 1985. Effect of R3+ ions on the structure and properties of lanthanum borate glasses. Journal American Ceramic Society 68 .641–645.

[12] Verwey, J. W. M., Imbusch, G. F., Blasse, G. 1989. Laser excited spectroscopy of Gd3+ ions in crystalline and glass borate hosts with

comparable composition. Journal Physics Chemistry Solids 50. 813–820.

[13] Dong, H. O. 2017. Shielding properties of 80TeO$_2$-5TiO$_2$-(15-x) WO$_3$-xAnOm glasses using WinXCom and MCNP5 code. Radiation Physics and Chemistry, 141 172-178.

[14] Mcalister, D. R. 2012. *Gamma-ray* attenuation properties of common shielding materials. University Lane Lisle.

[15] Nergiz, Y. Y. 2019. Nergiz. Gamma-ray Shielding Properties of Lithium Borate Glass Doped with Colemanit Mineral BEU Science Journal .8 (3) 762-771.

[16] Erkil, İ., Altınsoy , N., Karaaslan, İ. S. ¸ Bora A. 2016. Determination of Photon Mass Attenuation Coefficient for Some Phantom Materials using GATE Code and Comparison with Experimental and XCOM Data. International Journal of Nuclear and Radiation Science and Technology, 1 (2) 11-13.

[17] Özyurt, O., Altınsoy , N., Ş., Karaaslan, İ., Bora, A., Büyük, B., Eril, İ. 2018. Calculation of gamma-ray attenuation coefficient of some granite samples using a Monte Carlo simulation code, Radiation Physics and Chemistry 144. 271-275.

[18] Aral, İ. 2019. Investigation of Nuclear Shielding Capabilities of Alumina and Zirconia Based Ceramics with MCNP-X Code. Ağrı İbrahim Çeçen University, Master Thesis, Ağrı.

[19] COŞKUN, A., YİĞİTOĞLU, İ., TOPAKLI, H., & CETİN, B. (2023). Determination of the Radiation Shielding Performance of MoO2 Addition On PbO by Monte Carlo Simulation. In International Conference on Pioneer and Innovative Studies (Vol. 1, pp. 223-227).

[20] Tekin, H. O., Abouhaswa, A. S., Kilicoglu, O., Issa, S. A., Akkurt, I., & Rammah, Y. S. (2020). Fabrication, physical characteristic, and gamma-photon attenuation parameters of newly developed molybdenum reinforced bismuth borate glasses. Physica Scripta, 95(11), 115703.

[21] Alzahrani, J. S., Hessien, M., Alrowaili, Z. A., Kebaili, I., Olarinoye, I. O., Arslan, H., & Al-Buriahi, M. S. (2022). Fabrication and characterization of La2O3–Fe2O3–Bi2O3 nanopowders: Effects of La2O3 addition on structure, optical, and radiation-absorption properties. Ceramics International, 48(16), 22943-22952.