A theoretical study: radiation shielding features of polymer materials[*]

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Abstract

By using innovative approaches in material science and the artificial intelligence tools developed following these developments, it is possible to obtain information about materials that have not yet been produced or have only been produced as samples. Ionizing radiation is a type of radiation frequently used in industry and medicine, and its use requires taking precautions. These precautions consist of three rules: time, distance, and shielding. Within the scope of this study, the attenuation properties of polymeric materials using XCOM and PHY-X/PSD were investigated and compared, especially for shielding needs.

Keywords

Ionizing radiation, polymer, attenuation, XCOM, PHY-X/PSD

1. Introduction

Analysis of data using geometric modeling and computer-aided graphics tools in industrial areas reveals multivariate data structures that can form the basis of artificial intelligence applications [1]. Based on this, the material properties of light shielding materials developed for radiation protection in areas where ionizing radiation is used are determined using artificial intelligence tools and various programs. Ionizing radiation shielding has been a very important issue since the discovery of radiation in our lives. It is encountered in many different fields of work, especially in the environment and living health, as well as in the protection of electronic devices and space studies. Material development studies are being carried out to protect and preserve human beings from cosmic/space radiation, which occurs with the peaceful use of ionizing radiation and continues to exist naturally.The fact that polymer materials are open to development due to their structure and can be strengthened by adding particles with different properties shows that they are suitable for studies on weakening ionizing radiation. According to this reason, Poly (methyl methacrylate) (PMMA) polymer was preferred as a base material. The PMMA polymers have glassy properties, and their surface toughness is high. Especially, despite its high transparency, it has high defiance to ultraviolet rays and weather conditions, and it can be easily shaped under heat treatment are the reasons why PMMA polymer is preferred industrially [2]. The industrial areas where PMMA is of significant importance are quite diverse, especially in medical, electronic devices, automotive, optics, and furniture [3]. In this study, the linear attenuation coefficient of the composite PMMA/Borax material obtained by adding Borax to the Polymethyl methacrylate polymer was calculated using computer programs XCOM [4] and PHY-X/PSD [5] as a result of the interaction with ionizing gamma radiation. The XCOM program calculates only the mass attenuation coefficient, but the PHY-X/PSD is more practical than XCOM, as it calculates all

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radiation shielding parameters quickly and accurately. This is where the difference between the two programs comes from [5].

2. Materials

Polymethyl methacrylate polymer, formed by the polymerization of methyl methacrylate monomer, was supported by sodium decahydrate additive during the polymerization stage to obtain polymethyl methacrylate-borax composite [6]. This thermoplastic polymer-based composite is expected to absorb ionizing radiation.

Table 1
Chemical formulas of materials [6]

Material	Chemical Formula
Methyl methacrylate	$C_5H_8O_2$
Poly (methyl methacrylate)	$(C_5H_8O_2)_n$
Sodium decahydrate	$Na_2B_4O_7.10H_2O$

3. Theoretical Calculations

The linear attenuation coefficient (LAC), mass attenuation coefficient (MAC), half value layer (HVL), and tenth value layer (TVL) of the base material polymethyl methacrylate and PMMA/Borax composite were calculated. μ in the Lambert-Beer equation [7] indicates the linear attenuation coefficient and its unit is (cm^{-1}).

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

where, "I" is the intensity of gamma photons after the interaction, "I_0" is the intensity of gamma photons coming from the source and "x" is the thickness of the material.

Another way to define linear attenuation coefficient is the ratio of mass attenuation coefficient (cm^2/g) and material density (g/cm^3).

The other parameters half value layer and tenth value layer, represent material thicknesses that reduce the intensity of incoming gamma photons by half and one-tenth [8]. Equations 2 and 3 are obtained from the Lambert-Beer equation modification.

$$HVL = \frac{\ln 2}{\mu}, \tag{2}$$

$$TVL = \frac{\ln 10}{\mu}, \tag{3}$$

3.1. XCOM Program

The XCOM program was developed with support from the National Institute of Standards and Technology and calculates the mass attenuation coefficient depending on the material weight and radiation energy.

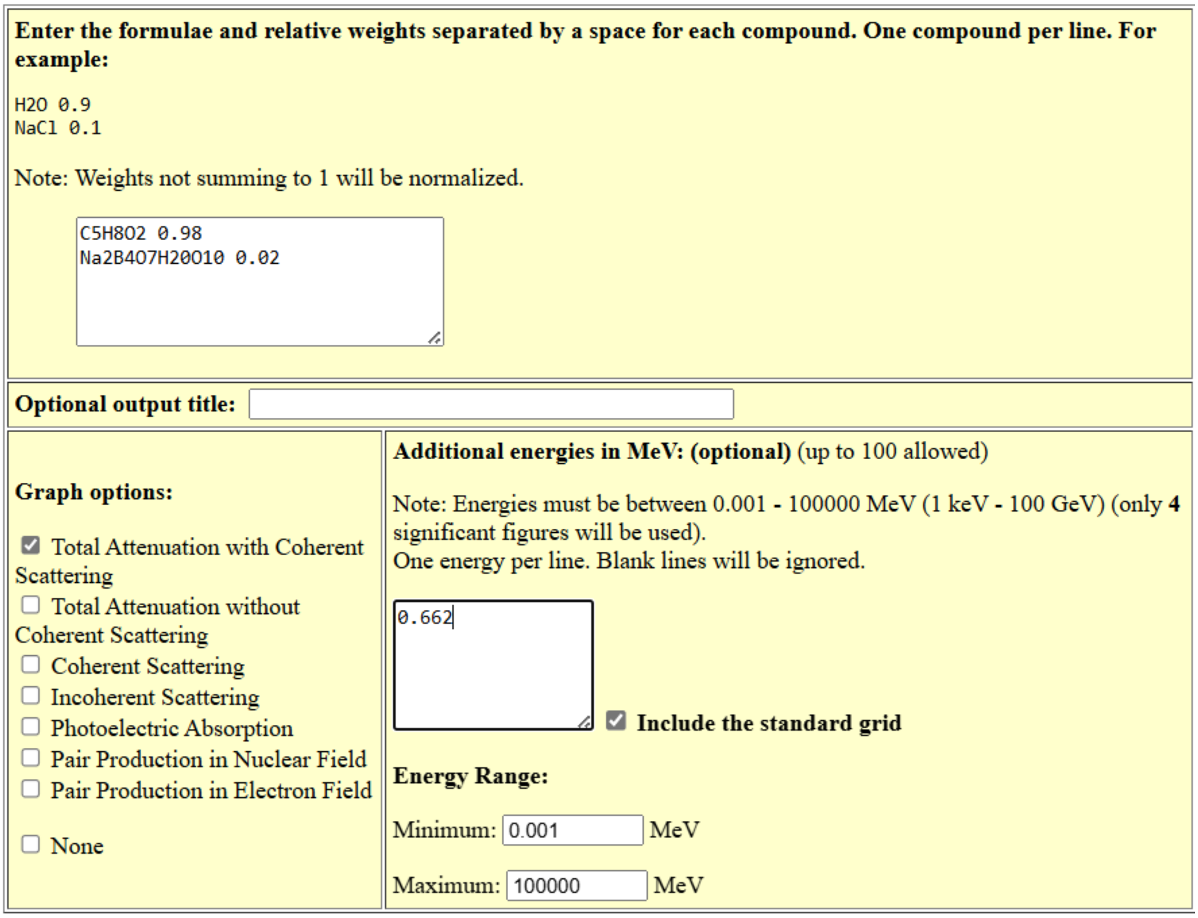

Figure 1: An example, XCOM program material formulas and radiation source energy input for 2% Borax doped Poly (methyl methacrylate).

Edge	(required) Photon Energy	Scattering		Photoelectric Absorption	Pair Production		Total Attenuation	
		Coherent	Incoherent		In Nuclear Field	In Electron Field	With Coherent Scattering	Without Coherent Scattering
	MeV	cm^2/g	cm^2/g	cm^2/g	cm^2/g	cm^2/g	cm^2/g	cm^2/g
	6.620E-01	9.994E-05	8.314E-02	5.374E-06	0.000E+00	0.000E+00	8.324E-02	8.314E-02

Figure 2: An example, XCOM program output (mass attenuation coefficient) for 2% Borax doped Poly (methyl methacrylate).

The above steps are repeated for all materials and radiation sources. In this above example, the Cs-137 gamma source's energy, 662 keV, was used. In addition to this example, the base PMMA, and 7% Borax doped PMMA were used. Linear attenuation coefficient, HVL, TVL calculations, and obtained from XCOM values are given next chapter.

3.2. PHY-X/PSD Program

The PHY-X/PSD program is more user-friendly than the XCOM program, and calculates all parameters of shielding like linear attenuation coefficient, mass attenuation coefficient, half value, and tenth value layer. This is a huge advantage for time-saving. Another difference between the two programs is that in the PHY-X/PSD program, material density and weight fraction must be given, while in the XCOM program, only the weight is important.

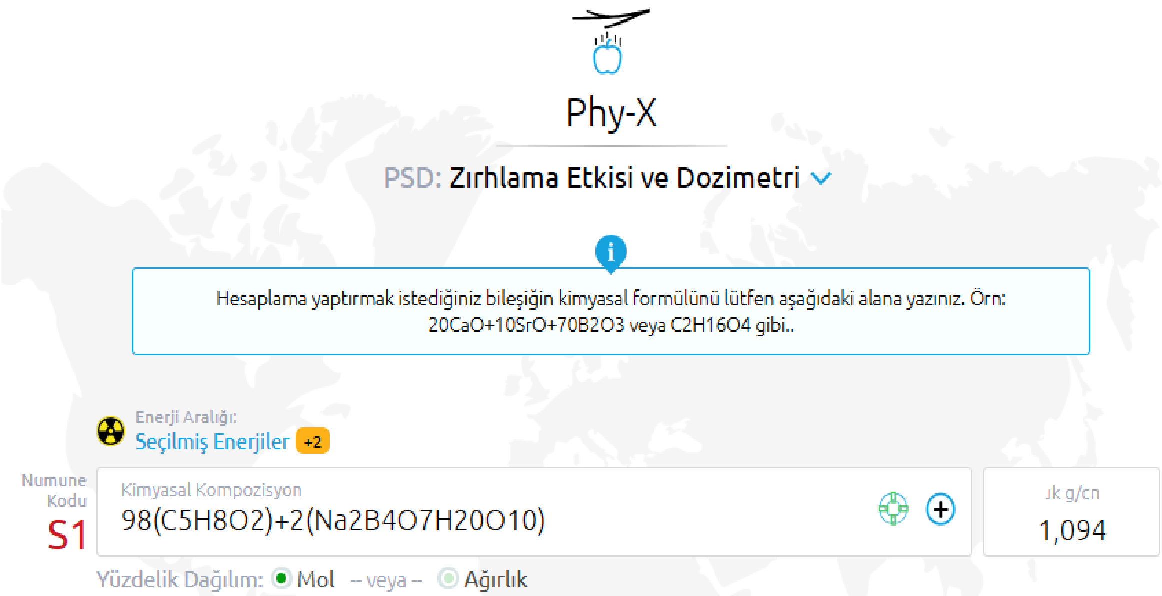

Figure 3: An example, PHY-X/PSD program input for 2% Borax doped Poly (methyl methacrylate) formula and density.

Figure 4: PHY-X/PSD program input for radiation source and energy.

The above steps run determining chemical formulas, density, weight fractions, and radiation sources. Transferring the calculation outputs to Excel can be considered as another advantage. At this point, transferring to Excel will make it easier to work on the results.

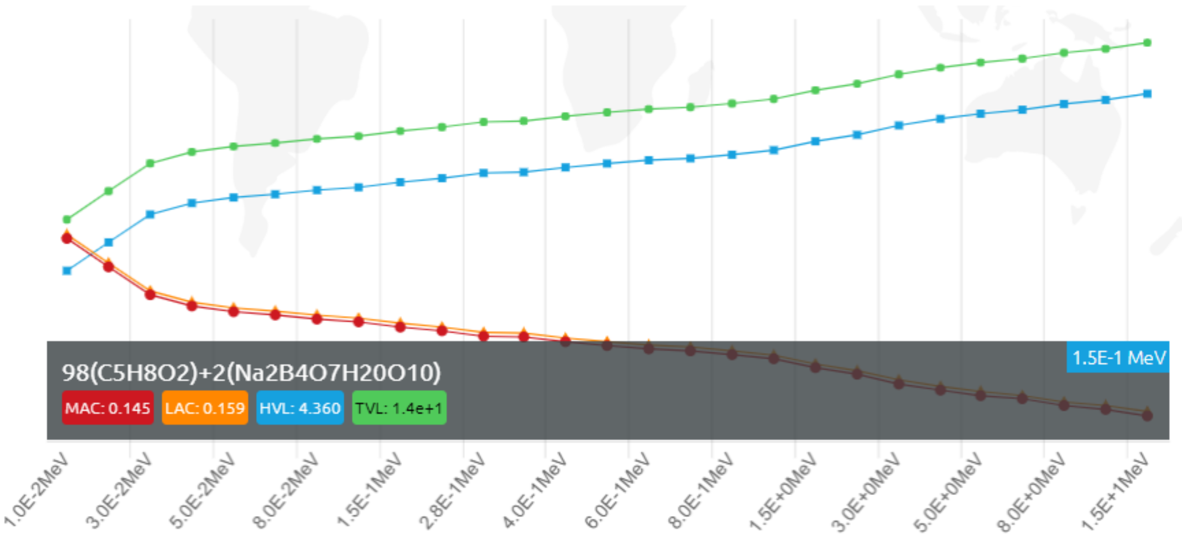

Figure 5: PHY-X/PSD program output graphic for all parameters.

After this, transferring to Excel;

Energy		**MAC**	**LAC**	**HVL**	**TVL**
MeV		*cm²/g*	*1/cm*	*cm*	*cm*
6,62E-01	*Cs (137)*	0,08310	0,09091	7,62436	25,32758

Figure 6: An example, PHY-X/PSD program Excel output for all parameters for 2% Borax doped Poly (methyl methacrylate).

4. Results

4.1. Mass attenuation coefficient

Table 2
Mass attenuation coefficient under 662 KeV Gamma photons of Cs-137

Samples	Density $\rho (g/cm^3)$	MAC (XCOM) μ/ρ (cm^2/g)	MAC (PHY-X) μ/ρ (cm^2/g)	Difference (‰)
PMMA	1.068	0.08331	0.08332	0.12
2% Borax doped	1.094	0.08324	0.08310	1.68
7% Borax doped	1.124	0.08309	0.08263	5.56

The mass attenuation coefficient gives information about the rate of photons removed per unit mass from absorber materials. Let’s keep on the linear attenuation coefficient results.

4.2. Linear attenuation coefficient

Table 3
Linear attenuation coefficient under 662 KeV Gamma photons of Cs-137

Samples	Density ρ(g/cm^3)	LAC (XCOM) μ (cm^{-1})	LAC (PHY-X) μ (cm^{-1})	Difference (‰)
PMMA	1.068	0.08897	0.08899	0.22
2% Borax doped	1.094	0.09106	0.09091	1.65
7% Borax doped	1.124	0.09339	0.09288	5.49

The linear attenuation coefficient is a constant that describes the extent to intensity of the beam decreases per unit of thickness. Both tables 2 and 3 show, that when the mass attenuation coefficient increases by doped effect, the linear attenuation coefficient decreases or opposites.

4.3. Half value layer and tenth value layer

Table 4
Half value layer and tenth value layer under 662 KeV Gamma photons of Cs-137

Samples	HVL (XCOM) (cm)	HVL (PHY-X) (cm)	TVL (XCOM) (cm)	TVL (PHY-X) (cm)
PMMA	7.79080	7.78907	25.8805	25.8747
2% Borax doped	7.61198	7.62436	25.2865	25.3276
7% Borax doped	7.42207	7.46270	24.6556	24.7905

5. Conclusion

When we look at the difference between the two programs, we can say that the differences do not even reach the level of ten per thousand and these differences can be ignored, therefore the programs are of a quality that replaces each other and even the PHY-X/PSD program is superior due to its advantages. This comparative examination shows that both programs can be used interchangeably and PMMA used as polymer and borax added can be used for gamma absorption. Certainly, the actual values of these theoretically evaluated examples will vary. However, the differences that are likely to be caused by many parameters such as material homogeneity, density, and impurity are expected to be quite small. The study shows that the PHY-X program gives faster results as an alternative to XCOM and GEANT-4 and that various results can be obtained with the additive material added to a polymer material. It is obtained to evaluate the approximate results of the composites to be produced before production by saving material. Geometric modeling has a high potential as a tool to represent system behavior with minimal projection requirements. Such a framework offers promising compatibility with artificial intelligence techniques aimed at optimizing material-aware system performance [9]. This study has emphasized that artificial intelligence and various computer programs have great importance in contributing to materials science and evaluating innovative approaches.

Declaration on Generative AI

During the preparation of this study, the authors used Grammarly software to identify and correct grammatical and spelling inaccuracies. Following this process, they undertook a meticulous review of the text, made the requisite revisions, and accepted whole responsibility for the final content of this publication.

References

[1] Gumen, O., Spodyniuk, N., Ulewicz, M., Martyn, Y. (2017). Research of thermal processes in industrial premises with energy-saving technologies of heating. Diagnostyka, 18.

[2] Forte, M. A., Silva, R. M., Tavares, C. J., & Silva, R. F. E. (2021). Is poly (Methyl Methacrylate) (PMMA) a suitable substrate for ALD?: A review. Polymers, 13(8), 1346. https://doi.org/10.3390/polym13081346

[3] Mehranpour, S. (2020). Comparison of beta, neutron and gamma attenuation properties of pmma/colemanite composites.

[4] Berger, M.J., Hubbell, J.H., 1987. XCOM: Photon Cross Sections Database, Web Version 1.2. National Institute of Standards and Technology, Gaithersburg, MD 20899, USA available at. http://physics.nist.gov/xcom.

[5] Şakar, E., Özpolat, Ö. F., Alım, B., Sayyed, M. I., & Kurudirek, M. (2020). Phy-X/PSD: development of a user friendly online software for calculation of parameters relevant to radiation shielding and dosimetry. Radiation Physics and Chemistry, 166, 108496. https://doi.org/10.1016/j.radphyschem.2019.108496

[6] Yigit, Y., Gul, F. B., Macun, C. H., & Baydogan, N. (2023). Optical development and density modification dependence in poly (methyl methacrylate) reinforced with borax microparticles. Journal of Polymer Research, 30(9), 359. https://doi.org/10.1007/s10965-023-03746-y

[7] Holburg, J., Figul, S., Charvat, A., Bluhm, H., Abel, B., Marowsky, G., ... & Mann, K. (2025). Soft X-Ray Absorption Spectroscopy With a Flat Liquid Jet in Vacuum Using a Table-Top Laser-Induced Plasma Source. X-Ray Spectrometry. https://doi.org/10.1002/xrs.3474

[8] Knoll, G. F. (2010). Radiation detection and measurement. John Wiley & Sons.

[9] Humen, O. M., Liaskovska, S. Ye., & Martyn, Ye. V. (2018). Sufficiency of projection images of 1-manifolds in *n*-dimensional state spaces of technical systems. *Applied Issues of Mathematical Modelling*, (1), 58–67.