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Comparison between MCNP5, Geant4 and experimental data for gamma rays attenuation of $PbO–BaO–B_2O_3$ glasses

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ABSTRACT

Monte Carlo simulations, MCNP5 and Geant4 codes were developed to investigate radiation shielding properties of xPbO–(50-x) BaO–50B2O3 (where $5 \leq x \leq 45$ mol%) consider to be glass systems. The mass attenuation coefficients were evaluated for different PbO concentration in the glass samples for varies photon energies of 0.356, 0.662, 1.173 and 1.332 MeV. The obtained mass attenuation coefficient values used to calculate half-value layer, effective atomic number, and electron density. The simulation parameters were compared with experimental data. Results show that the simulation results of mass attenuation coefficients for all PbO concentrations were generally in good agreement with experimental results, however, mass attenuation coefficient values calculated using Geant4 were slightly lower than MCNP5 and experimental data on the low energy of 0.356 MeV. The results obtained from MCNP5 and Geant4 codes might be able to assessment mass attenuation for different glass systems. Furthermore, gamma ray, fast neutron and charged particle interaction for the glass systems were studied using buildup factors, fast neutron removal cross sections and ranges respectively.

1. Introduction

The destructive effects of X-ray and gamma radiation are well known in these days. The radiation technology has been used in several areas such as medicine, factories, and food production, however, it is needed to protect against the risky effects of ionizing radiation not only for human but also for the environment [1, 2, 3, 4]. Any radiation leakage may interact with the human body and cause direct harm to vital organs such as blood, bones and soft tissues. Hence, it was essential to develop new radiation protection materials against photons or charged particles such as alpha, beta and gamma radiations, to lose all their energy when interacting with such materials [5]. X-ray and gamma rays can penetrate and interact with all leaving materials; therefore, it can be considered as the greatest dangerous radiations in the case of radiation leakage and need special materials to stop it.

To measure the absorption of gamma radiation per unit mass, mass attenuation coefficient (μm) is used. It is considered to be the main factor to describe several extra factors of shielding effects and radiation interaction with matter [6, 7, 8]. Almost all elements have extensive data in the literature relevant to mass attenuation coefficient scattering and cross-section. Most of the output data are associated with the theoretical data used by computing software such as XCOM, MCNP and Geant4 programs [9, 10].

Monte Carlo Neutron and Photon (MCNP) or Monte Carlo simulation is a tool created using mathematical Monte Carlo method to answer the transport equation to study radiation interactions with the matter was developed by the Los Alamos National Laboratory. It can work on many ways of radiation exposure and can use electrons, photons, and neutrons as a radiation source [11, 12, 13]. MCNP is an operational tool to estimate radiation interaction parameters in different sorts of mixtures and compounds for shielding and energy admission in human organs and tissues using physics models for nuclear cross-section and particle interactions libraries and can be an [14].

Geant4 code is created using the C++ programming language which allows the user to develop modules to define a primary particle generator, detector geometry, and physics processes, models. Furthermore, Geant4 can state electromagnetic and decay physics as well as physics processes models include ionization, scattering, annihilation, photoelectric, Compton and pair production. Although the Geant4 simulation toolkit works on wide-range energy, it also provides flexibility and ease of use.

The experimental structure of the Geant4 simulation containing a

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Table 1
Chemical composition, density, and thickness of the investigated glass samples.

Sample No.	Composition (mole %)			Density ρ (g/cm^3)	Thickness (cm)
	PbO	BaO	B_2O_3		
1	5	45	50	4.318 ± 0.043	0.523
2	10	40	50	4.460 ± 0.045	0.633
3	15	35	50	4.602 ± 0.046	0.752
4	20	30	50	4.744 ± 0.047	0.834
5	25	25	50	4.886 ± 0.049	0.912
6	30	20	50	5.028 ± 0.050	1.254
7	35	15	50	5.170 ± 0.051	1.321
8	40	10	50	5.312 ± 0.053	1.435
9	45	5	50	5.454 ± 0.055	1.511

radioactive beam impacting on material is similar to the scintillation detector process, photon attenuation is calculated by simulating all related physical procedures and relations. Reference data of electromagnetic processes for the Geant4 model have been extracted from the National Institute of Standards and Technologies (NIST) database [15, 16].

There is several works dealing with the determination of mass attenuation coefficients (μm) for different glass systems [17, 18, 19, 20, 21, 22, 23, 24, 25]. Most of the previously reported works for determining the μm have been carried out experimentally. The present work aimed to determine the μm of glass materials by Monte Carlo simulation and Geant4. In this study, experimental data [1] were used to test the validity of MCNP and Geant4 simulations to confirm its radiation interactions of xPbO–(50-x) BaO–50B2O3 (where 5 ≤ x ≤ 45 mol%) glass systems. It is known that borate glasses have good thermal stability, high chemical resistance, low melting point, and low viscosity. Incorporating heavy metal oxides like BaO and PbO to the borate glasses increases the density of the glass sample and this enhances the radiation shielding properties for the glass sample. The two codes were applied in calculating mass attenuation coefficients for varies photon energies of 0.356, 0.662, 1.173 and 1.332 MeV and compared with the experimental measurements. Besides, the obtained μm values then used to calculate other related parameters such as half-value layer (HVL), effective atomic number (Zeff) and electron density (Nel). Moreover, by using the G-P fitting method, the buildup factors (EBF and EABF) have been calculated for the investigated glass samples. This type of study presents an alternative method to experiment for the development of standards and guidelines for different glass systems and help in testing samples in order to save materials and efforts.

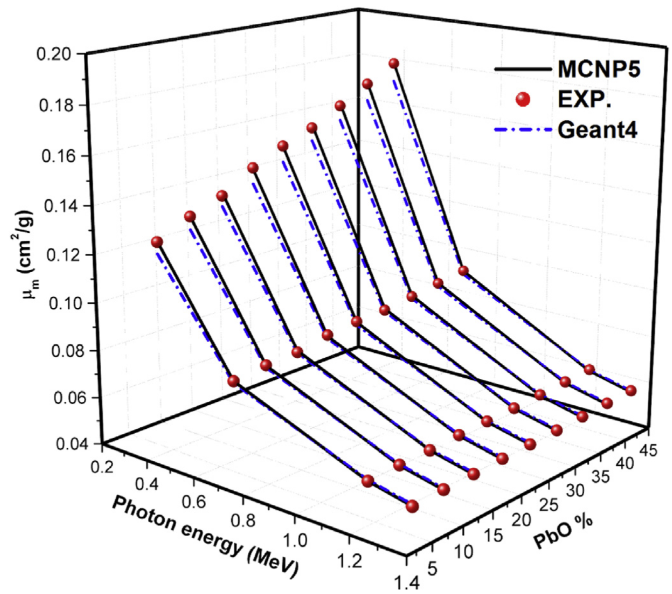

Fig. 1. Comparison of mass attenuation coefficients calculated a different PbO concentration using MCNP5 and Geant4 codes with respect to experimental values.

2. Materials and methods

Ternary PbO–(50-x) BaO–50B2O3 (where 5 ≤ x ≤ 45 mol%) glass system were considered to be tested using gamma ray, charged particle interaction and fast neutron using different parameters such as mass attenuation coefficients (μm), half-value layer (HVL), effective atomic number (Zeff), electron density (Nel), buildup factors, fast neutron removal cross sections (∑R) and ranges (R). The chemical compositions and densities of the investigated samples are given in Table 1. The studied glass density was adopted from Ref. [1].

Table 2
Comparison of mass attenuation coefficients (cm^2/g) of the selected glasses obtained using MCNP5 and Geant4 simulation and experimental results.

PbO %	Mass attenuation coefficient (μ_m) (cm^2/g)									
	0.356 MeV					0.662 MeV				
	Exp.	MCNP5	RD[a]	Geant4	RD[b]	Exp.	MCNP5	RD[a]	Geant4	RD[b]
5	0.12598	0.12636	0.022	0.1211	-0.276	0.07769	0.07773	0.010	0.0769	-0.199
10	0.13271	0.13285	0.008	0.1272	-0.312	0.07929	0.07917	-0.030	0.0783	-0.251
15	0.13776	0.13933	0.089	0.1333	-0.253	0.07992	0.08063	0.180	0.0796	-0.080
20	0.14622	0.14580	-0.024	0.1394	-0.387	0.08251	0.08208	-0.109	0.081	-0.382
25	0.15235	0.15230	-0.003	0.1455	-0.388	0.08377	0.08353	-0.059	0.0823	-0.371
30	0.15721	0.15877	0.088	0.1516	-0.318	0.08436	0.08500	0.162	0.0837	-0.166
35	0.16404	0.16525	0.069	0.1577	-0.360	0.08602	0.08645	0.109	0.0851	-0.232
40	0.17111	0.17176	0.037	0.1638	-0.414	0.08779	0.08791	0.029	0.0864	-0.352
45	0.17782	0.17825	0.024	0.1699	-0.449	0.08938	0.08936	-0.004	0.0878	-0.399
	1.173 MeV					1.33 MeV				
5	0.05516	0.05518	0.016	0.0556	0.373	0.05121	0.05131	0.093	0.0519	0.684
10	0.05570	0.05554	-0.136	0.0559	0.168	0.05171	0.05160	-0.108	0.0522	0.487
15	0.05586	0.05590	0.034	0.0563	0.374	0.05197	0.05190	-0.070	0.0525	0.532
20	0.05654	0.05626	-0.234	0.0567	0.136	0.05240	0.05219	-0.209	0.0528	0.395
25	0.05679	0.05662	-0.143	0.057	0.178	0.05257	0.05248	-0.092	0.0531	0.524
30	0.05709	0.05699	-0.086	0.0574	0.260	0.05293	0.05278	-0.152	0.0533	0.370
35	0.05763	0.05735	-0.233	0.0578	0.147	0.05336	0.05307	-0.292	0.0536	0.236
40	0.05823	0.05771	-0.436	0.0581	-0.111	0.05386	0.05337	-0.496	0.0539	0.036
45	0.05871	0.05807	-0.536	0.0585	-0.177	0.05425	0.05366	-0.585	0.0542	-0.046

RD[a] is the relative difference between MCNP5 and experiment.
RD[b] is the relative difference between Geant4 and experiment.

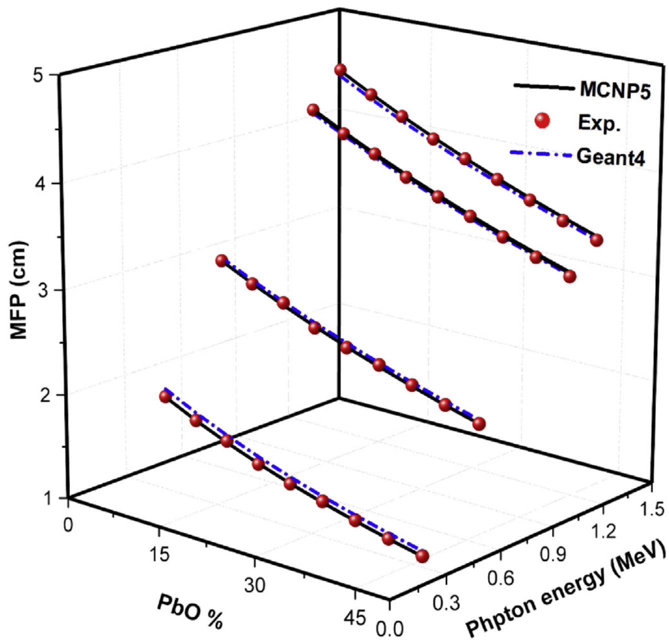

Fig. 2. Comparison of mean free path calculated a different PbO concentration using MCNP5 and Geant4 codes with respect to experimental values.

2.1. Monte Carlo methods

2.1.1. MCNP5 code

MCNP code version 5 was used in this study using continuous energy nuclear and atomic data libraries, its source is an isotropic point source and was defined by particle type, exact energy, position, and direction. Simulated geometry was the same as used in the previous study [26]. The narrow beam photon was obtained by two collimators between the source and the sample. Sample thickness has been placed to be 1 cm and at a distance of 100 cm from the source. Also, the detector was placed 50 cm far from the source and of only 1 cm thickness. All these geometrical parameters were introduced to MCNP software surface and cell card.

All MCNP5 simulated data were recorded using tally card F4. Using this tally card, particle flux in a cell was calculated and the output results were represented by particles/cm2. Tally energy card was used to record photon energy emitted by the source data, as the narrow beam photon is composed of non-colliding photons. The number of starting particles run is 108.

2.1.2. Geant4 code

Geant4 [15] is a tool kit to simulate the passage of particles through matter using cross-sections up-to-date data from experimental particles reactions. Geant4 is widely used including applications in high energy, nuclear and accelerator physics, as well as studies in medical and space science. In 1993 two research groups in particle physics at CERN, Geneva, Switzerland, and KEK Center, Tsukuba, Japan, have the first

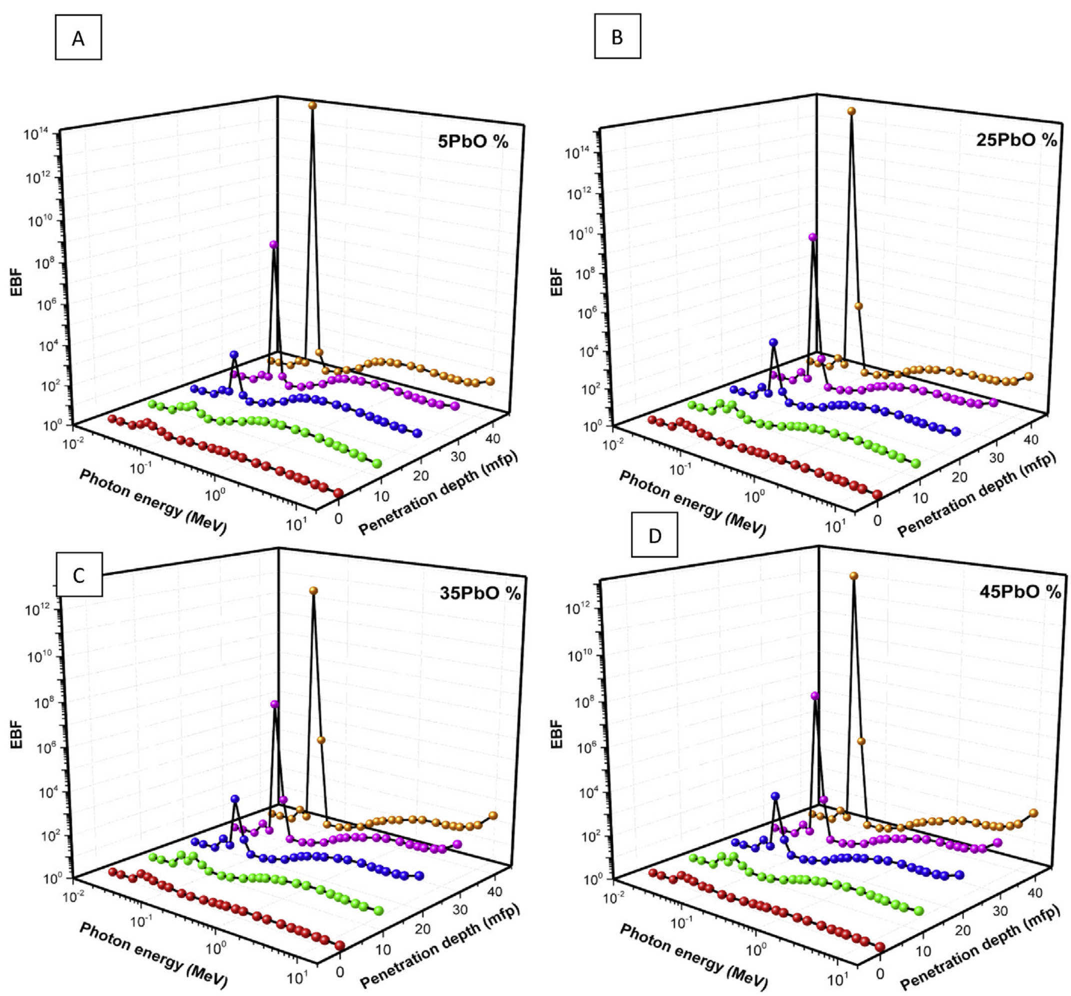

Fig. 3. Variations of exposure buildup factors with photon energy for glasses the energy region 0.015–15 MeV at 1, 10, 20, 30 and 40 mfp for (A) 5PbO% (B) 25PbO% (C) 35PbO% and (D) 45PbO%.

Table 3
Comparison of the effective atomic number (Z_{eff}) and electron density (N_{el}) of the selected glasses obtained using MCNP5 and Geant4 simulation and experimental results.

PbO %	0.356 MeV						0.662 MeV					
	Z_{eff}			$N_{el}\times10^{23}$			Z_{eff}			$N_{el}\times10^{23}$		
	MCNP5	Exp.	Geant4	MCNP5	Exp.	Geant4	MCNP5	Exp.	Geant4	MCNP5	Exp.	Geant4
5	12.40	12.21	12.02	3.15	3.10	3.06	11.74	11.64	11.59	2.99	2.96	2.95
10	12.76	12.44	12.23	3.23	3.15	3.10	11.94	11.76	11.70	3.02	2.98	2.96
15	13.11	12.60	12.44	3.30	3.17	3.13	12.15	11.83	11.81	3.06	2.98	2.97
20	13.46	12.87	12.64	3.37	3.22	3.17	12.35	12.02	11.93	3.10	3.01	2.99
25	13.79	13.05	12.83	3.44	3.25	3.20	12.55	12.12	12.04	3.13	3.02	3.00
30	14.11	13.18	13.01	3.50	3.27	3.23	12.76	12.19	12.15	3.17	3.02	3.01
35	14.43	13.37	13.18	3.56	3.30	3.26	12.96	12.32	12.26	3.20	3.04	3.03
40	14.73	13.56	13.35	3.62	3.33	3.28	13.17	12.45	12.37	3.24	3.06	3.04
45	15.03	13.73	13.52	3.68	3.36	3.30	13.38	12.57	12.48	3.27	3.07	3.05
	1.173 MeV						1.33 MeV					
5	11.53	11.42	11.46	2.93	2.90	2.91	11.49	11.39	11.45	2.92	2.90	2.91
10	11.67	11.51	11.53	2.95	2.91	2.92	11.62	11.48	11.53	2.94	2.90	2.92
15	11.81	11.57	11.61	2.97	2.91	2.92	11.76	11.55	11.60	2.96	2.91	2.92
20	11.95	11.67	11.69	2.99	2.93	2.93	11.90	11.64	11.68	2.98	2.92	2.93
25	12.10	11.74	11.76	3.02	2.93	2.93	12.04	11.70	11.75	3.00	2.92	2.93
30	12.24	11.81	11.84	3.04	2.93	2.94	12.18	11.78	11.82	3.02	2.92	2.93
35	12.39	11.91	11.92	3.06	2.94	2.94	12.33	11.87	11.89	3.04	2.93	2.94
40	12.54	12.00	11.99	3.08	2.95	2.95	12.48	11.97	11.97	3.07	2.94	2.94
45	12.70	12.09	12.08	3.10	2.96	2.95	12.63	12.05	12.05	3.09	2.95	2.95

ideas for the need to modify the Geant3 version, written in FORTRAN, to use new programming techniques within C++ and its object-oriented technology. In 1994 both groups merged their work and the geant4 proposal was submitted to CERN's Detector Research and Development Committee under the research and development project RD44 [27]. Now, Geant4 is a Mega-Collaboration from all over the world that make it the best program to simulate the interaction of particles with matter. Geant4, in contrast with Geant3, can track particles to zero energy range

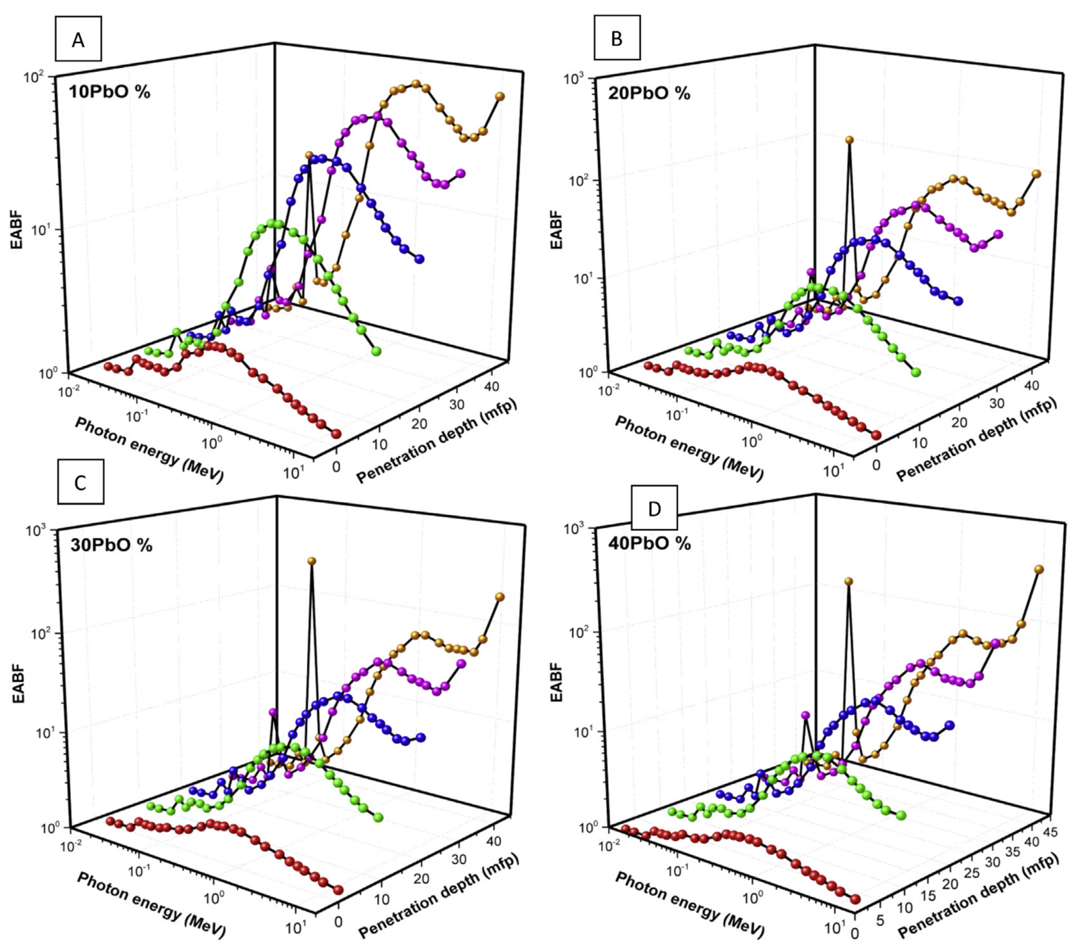

Fig. 4. Variation of energy absorption buildup factor (EABF) with photon energy for glasses the energy region 0.015–15 MeV at 1, 10, 20, 30 and 40 mfp for (A) 10PbO% (B) 20PbO% (C) 30PbO% and (D) 40PbO%.

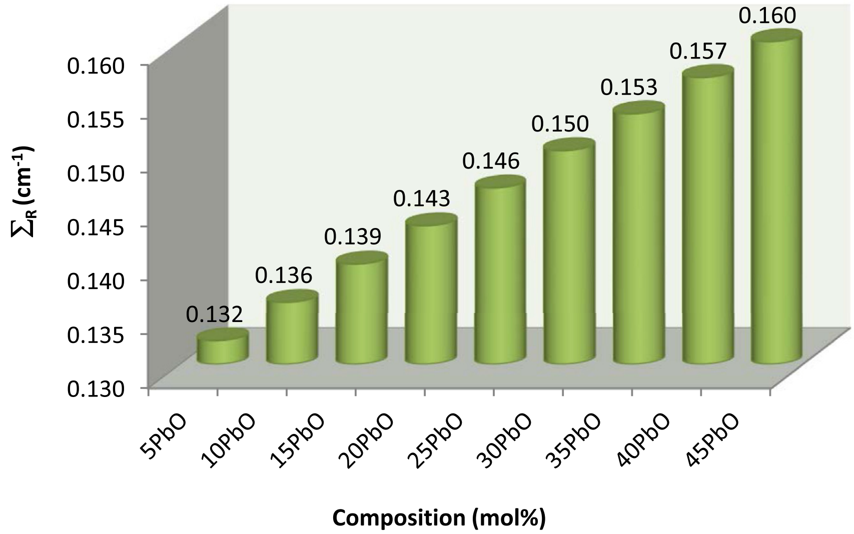

Fig. 5. Variation of removal cross-section for fast neutron versus composition of PbO.

using new experimental and theoretical development in electromagnetic and hadronic processes. In Geant4 there are two extensions physics lists for the interaction of photons at low energy, below 1 GeV, including Photoelectric process and Compton scattering alow energy and photon bremsstrahlung and conversion at high energy: these are the Penelope and Livermore ElectroMagnetic models. Geant4 electromagnetic processes were used to study shielding of photons (X-rays) with by xPbO–(50-x) BaO–50B2O3 (where $5 \leq x \leq 45$ mol%) glass systems where x is the proportion of PbO in the glass.

Table 4
Calculation values of the fast neutron effective removal cross-sections for the investigated glass samples.

Elements	W_i	$\sum_{(R/\rho)}$ (cm^2/g)	ρ (g/cm^3)	$\sum_R$ (cm^{-1})
5PbO–45BaO–50B$_2$O$_3$				
B	0.155285	0.0575	2.340000	0.008929
O	0.395256	0.0405	0.001429	0.016008
Ba	0.403043	0.0129	3.594000	0.005199
Pb	0.046416	0.0104	11.34200	0.000483
Total				**0.1322**
10PbO–40BaO–50B$_2$O$_3$				
B	0.155285	0.0575	2.340000	0.008929
O	0.393622	0.0405	0.001429	0.015942
Ba	0.358260	0.0129	3.594000	0.004622
Pb	0.092832	0.0104	11.34200	0.000965
Total				**0.1358**
15PbO–35BaO–50B$_2$O$_3$				
B	0.155285	0.0575	2.340000	0.008929
O	0.391989	0.0405	0.001429	0.015876
Ba	0.313478	0.0129	3.594000	0.004044
Pb	0.139248	0.0104	11.34200	0.001448
Total				**0.1394**
20PbO–30BaO–50B$_2$O$_3$				
B	0.155285	0.0575	2.340000	0.008929
O	0.390356	0.0405	0.001429	0.015809
Ba	0.268695	0.0129	3.594000	0.003466
Pb	0.185664	0.0104	11.34200	0.001931
Total				**0.1430**
25PbO–25BaO–50B$_2$O$_3$				
B	0.155285	0.0575	2.340000	0.008929
O	0.388722	0.0405	0.001429	0.015743
Ba	0.223913	0.0129	3.594000	0.002888
Pb	0.232079	0.0104	11.34200	0.002414
Total				**0.1465**
30PbO–20BaO–50B$_2$O$_3$				
B	0.155285	0.0575	2.340000	0.008929
O	0.387089	0.0405	0.001429	0.015677
Ba	0.179130	0.0129	3.594000	0.002311
Pb	0.278495	0.0104	11.34200	0.002896
Total				**0.1499**
35PbO–15BaO–50B$_2$O$_3$				
B	0.155285	0.0575	2.340000	0.008929
O	0.385456	0.0405	0.001429	0.015611
Ba	0.134348	0.0129	3.594000	0.001733
Pb	0.324911	0.0104	11.34200	0.003379
Total				**0.1533**

2.2. *Fundamental shielding parameters*

The fundamental quantities describing radiation attenuation through the materials are mean free path (MFP), effective atomic number (Zeff), electron density (Nel), buildup factors for photons, a removal cross-section for neutron and projected ranges for protons and heavy ions. For the detailed knowledge on calculations of the different shielding parameters, we may refer to our recent studies [1, 3, 5, 8, 28, 29, 30, 31, 32, 33, 34, 35].

3. Results and discussion

The mass attenuation coefficients at different PbO concentrations were calculated using two simulation codes (Geant4 and MCNP5) at four different photon energies, 0.356, 0.662, 1.173 and 1.332 MeV. Results were compared with the experimental values that were obtained in the lab [1]. The results are exhibited in Fig. 1. Fig. 1 shows that the simulated results of mass attenuation coefficients for all PbO concentrations at the selected energies were generally in good agreement with experimental results, however, mass attenuation coefficient values calculated using Geant4 were slightly lower than MCNP5 and experimental data at the low energy of 0.356 MeV. Besides, Fig. 1 shows increase in the mass attenuation coefficient values as the concentration of PbO increases. Also, it has been noticed that the mass attenuation coefficient recorded increasing as the PbO concentration increased in the low energies compared to higher energies. Besides, MCNP5, Geant4 and experimental results of mass attenuation coefficient values with photon energies are listed in Table 2. The relative difference between MCNP5 and experiment and the relative difference between Geant4 and experiment are also shown in Table 2. It was found that the mass attenuation coefficient values obtained by MCNP5 and Geant4 at all PbO concentrations were almost similar to experimental results, the maximum deviation was found in the difference between Geant4 and an experiment was 0.684 at an energy of 1.33 MeV.

Using the mass attenuation coefficient values presented in Fig. 1 the mean free path (MFP) have been evaluated and the results are shown in Fig. 2. As can be seen from Fig. 2, MCNP5 and Geant4 simulation results are in satisfactory agreement with the experimental values. On the other

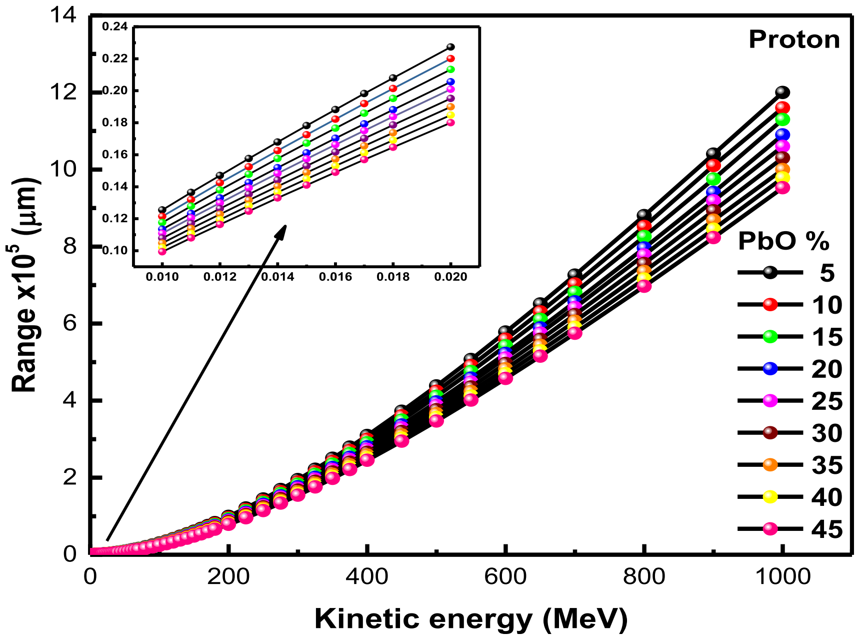

Fig. 6. Projected ranges of the glasses for proton interaction in the energy region 10 keV to 1 GeV.

hand, the mean free path (MFP) decreased as the concentration of PbO increases at all four energies for the Geant4, MCNP, and experimental results. With the increase of PbO concentration, the density of the selected glasses is increasing, hence the MFP decreases. Further, it is seen from Fig. 2 that the photon with low energy loses its energy in a short distance, whereas at high energy photon needs a long distance to lose their energy. In addition to this, it is obvious that photon loses its energy in a short distance for a glass contains higher PbO content than the other and the results are shown in Fig. 3.

The mass attenuation coefficients obtained by MCNP5, Geant4 codes and from the experimental data also used to calculate the effective atomic number (Zeff) and electron density (Nel) of the investigated glasses. The results are collected and listed in Table 3. It can be seen that the Zeff and Nel increased with increasing the concentration of PbO in glasses. Also, it was observed that the simulation processes using Geant4 and MCNP5 were in good agreement with the experimental data.

The variation in the exposure buildup factors (EBF) has been shown in Fig. 4 for 5, 25, 35 and 45% mol. PbO concentrations (as in example) in the energy range from 0.015 to 15 MeV at penetration depths 1, 5, 10, 20, 30 and 40 mfp. The same shape was found for the remaining glass samples. Studying buildup factors of the PbO glasses will give a better understanding to design and synthesize new radiation shielding materials.

Fig. 4 shows that the values of EBF were small in low energies region and increases as the photon energy and penetration depth increase, with a very sharp peak at 80 keV, corresponding to K-edge absorption of Pb, at all penetration depths.

The maximum and the minimum EBF value of PbO concentrations

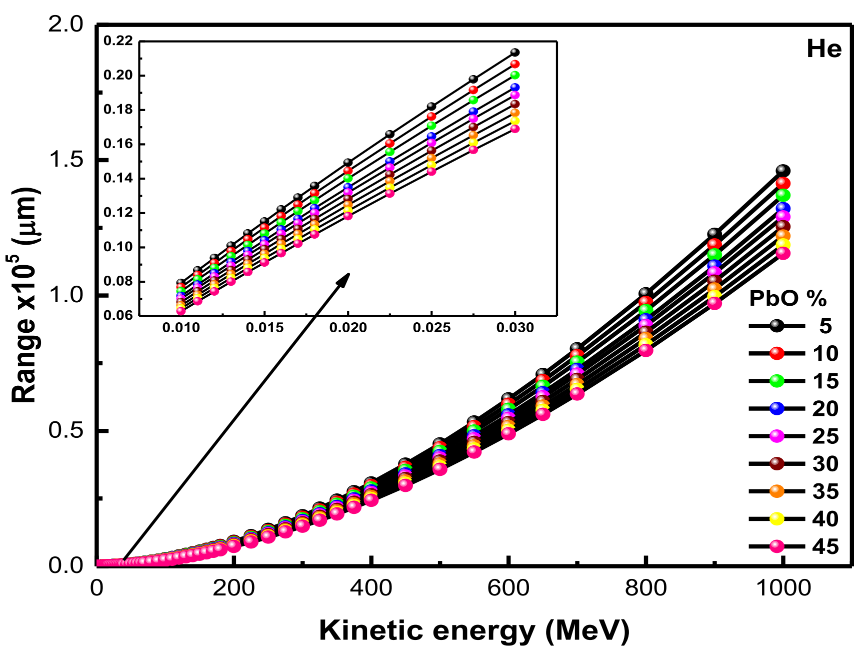

Fig. 7. Projected ranges of the glasses for He interaction in the energy region 10 keV to 1 GeV.

were found to be in the intermediate photon energy, and low and high energies regions respectively. The difference tendency of the build-up factors is detected compared to the photon energy of 3 MeV. On the other hand, the build-up factors found to be small in low energy as the photons are absorbed by photoelectric absorption, however, it was slowly increased due to Compton multiple scattering in the intermediate energy. And lastly reduces in the high energy region due to the pair production process. The variation of energy absorption buildup factor (EABF) with incident photon energy is shown in Fig. 4 for 10, 20 30, and 40% mol. PbO concentrations. It can be seen from Fig. 4 that the variation of EABF is similar to the variation of EBF with photon energy and the difference is only in their magnitudes.

Fig. 5 shows the variation of the removal cross-section for fast neutron ($\sum R$) of the ternary glass system xPbO–(50-x) BaO–50B2O3 and PbO mol.% concentration and exact values were collected in Table 4. It is seen from Fig. 5 that the removal cross-section for fast neutron increases with increase in PbO content in the composition range from 5 to 45 mol% PbO. This indicates that samples with higher PbO concentrations are significantly responsible for removal fast neutron more than samples with low PbO concentrations. The $\sum R$ of the present glasses are higher than those reported of ordinary concrete, hematite serpentine concrete [36].

SRIM database was used to simulate charged particle range. The average value of the depth to which a charged particle will penetrate upon slowing down to rest is known as projected ranges of heavy ions to represents the effect of the shielding material, in this studied glass samples the projected ranges were shown in Figs. 6 and 7. The projected range of the heavy charged particles tends to decrease when the Z of the ion increases, therefore, better radiation shielding came with the low projected value ranges. The 5PbO–45BaO–50B2O3 glass sample shows a high range of heavy charged particles, and the lowermost values of the total energy region were found in 45PbO–5BaO–50B2O3 glass sample.

4. Conclusion

The MCNP5 and Geant4 codes were used to determine μm, HVL, Zeff, and Ne for ternary glass system PbO–(50-x) BaO–50B2O3 (where $5 \leq x \leq 45$ mol%) at 0.356, 0.662, 1.173 and 1.332 MeV photon energies. The results of μm of the selected glasses were found comparable with the experimental results. Also, it was found that μm, Zeff, and Ne values have been increased as the concentration of PbO increases in the glass composition. Besides, the present glass system was investigated against fast neutron as well as proton and He interaction. The results indicated that samples with higher PbO concentrations are significantly responsible for removal fast neutron more than samples with low PbO concentrations. Besides, the projected range of the heavy charged particles tends to decrease when the Z of the ion increases, therefore, better radiation shielding came with the low projected value ranges. The 5PbO–45BaO–50B2O3 glass sample shows a high range of heavy charged particles, and the lowermost values of the total energy region were found in 45PbO–5BaO–50B2O3 glass sample.

The present work suggests that both MCNP5 and Geant4 codes are both appropriate to be utilized as an alternative and reliable method as the experiment in cases such as unavailable or expensive lab materials or hard to be conducted in some research premises.

Declarations

Author contribution statement

Mohammad Almatari: Conceived and designed the experiments; Analyzed and interpreted the data; Wrote the paper.

Shams A.M. Issa, M. G. Dong, Rachid Ayad: Conceived and designed the experiments; Performed the experiments; Wrote the paper.

M. I. Sayyed: Conceived and designed the experiments; Contributed reagents, materials, analysis tools or data; Wrote the paper.

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Competing interest statement

The authors declare no conflict of interest.

Additional information

No additional information is available for this paper.

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