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Photon attenuation computational software tools - A comparative study

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ABSTRACT

Various photon attenuation software tools are being used widely by researchers to evaluate the radiation shielding parameters of the elements/compounds/composites theoretically. Attempts are being made by a few researchers to update and develop software tools of these kinds. However, the efficacy of these tools in terms of their comparison is yet to be explored. Thus, an attempt has been made in the present study to compare & explore the best tool among the widely used and most trusted tools, such as Phy-X, XCOM, FFAST and XMuDat photon attenuation databases, to evaluate the shielding parameters of PVA-based composites filled with bismuth and tungsten, and also for materials such as bismuth, tungsten, gold, copper, platinum, lead and barite. Careful analysis of the data obtained computationally and experimentally shows that, although the Phy-X tool provides various shielding parameters with multiple choices in the selection of energy range, it is noticed that this tool needs to be figured out for obtaining the absorption edges of the composites of interest precisely. The XCOM database provides sharp absorption edges; however, this tool gives multiple values of mass attenuation coefficients corresponding to a particular absorption edge energy. On the other hand, The FFAST tool provides sharp absorption edges along with X ray fine structure. However, the tool restricts to work with elements and compounds in the energy range 1 keV–433 keV, which limits the utilization of this tool. Furthermore, the XMuDat tool has a limiting option to work with the materials available in its library/database and provides the mass attenuation coefficient and four other parameters. However, the XMuDat provides a large number of data points, which helps to identify any minute deviation in the values of the parameters. Therefore, the present study suggests that the XMuDat tool is much more advantageous and reliable than the other tools for the detailed study of various radiation shielding parameters.

1. Introduction

To evaluate theoretically the material of interest towards gamma ray attenuation, researchers widely use various photon attenuation software tools. Few studies have attempted to compare the available tools to the extent of comparing the number of parameters and the energy range provided by the tools [1,2]. Numerous studies have been conducted and reported on gamma ray shielding aspects of variety of materials. A significant number of these studies have focused on glass systems and composite materials. In a detailed study by Kaur et al., various heavy metal oxide glasses (^{56}Ba, ^{64}Gd, ^{82}Pb, ^{83}Bi) were analysed for their gamma ray shielding properties. The study took into account data from different researchers and recalculated the attenuation parameters using XCOM [3]. Meanwhile, Sopapan et al. evaluated the gamma attenuation properties of recycled glass from discarded CRTs using XCOM. They found that these glass systems performed better than ferrite concrete [4]. Kumar et al. have assessed the ability of $PbO + WO_3 + Na_2O + MgO$ doped borate glass systems to shield gamma rays using XCOM [5]. Mustafa Çaglar et al. have evaluated the $Na_2Si_3O_7$ glass system for attenuating gamma rays using XCOM [6]. Shielding efficiency of the Bi_2O_3 and PbO-loaded BaO glass system using XCOM and XMuDat tools was evaluated by Bhageri et al. [7]. A review study was conducted by More et al. on the synthesis of polymeric composite materials. The study focused on the role of nanofillers in enhancing radiation shielding

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efficiency. XCOM was used to assess the effectiveness of these material [8]. Harish et al. have evaluated the gamma shielding ability of lead oxides loaded isophthalic resin composites using XCOM and XMuDat [9]. In addition to these glass and composite polymer systems, other studies have also been conducted. For example, Dong et al. have assessed the shielding behavior of the material from chambersite (is a manganese borate mineral with formula $Mn_3B_7O_{13}Cl$) deposits in China using XCOM and Phy-X/PSD [10]. The gamma-ray attenuation properties of gypsum plaster using XMuDat have been evaluated by Vasconcelos et al. [11]. Tuissi et al. studied the substitution of Ti with rare earth elements and used the XMuDat tool for computational evaluation [12]. Vishwanath et al. assessed the shielding properties of low Z materials using XCOM and XMuDat [13]. These studies indicate widespread use of the tools mentioned. Olukotun et al. investigated the gamma ray shielding effectiveness of clay-polyethylene composites using EGS5, XCOM and Phy-X/PSD [14]. Aygun et al. analysed the radiation protection capability of Rene alloys (Ni:57%, Mo:15–17%, Cr:15.5–16.5%, Fe:4–7%; compositions differ for different alloy series such as Rene 80, 88 and 90) using Phy-X/PSD [15]. Yonca Yahsi ÇElen evaluated the gamma-ray shielding properties of various materials, including PLA, ABS, PETG, TPEs and PA for medical dosimeter using Phy-X/PSD [16]. Researchers have found that the computationally and experimentally obtained data are in good agreement. Therefore, it is important to conduct a direct comparative study of the data obtained using these tools (XCOM, XMuDat, FFast and Phy-X).

Among the tools mentioned, the XMuDat database provides four shielding parameters along with mass attenuation coefficients. On the other hand, the XCOM database provides only the mass attenuation coefficient of the desired composites. Similarly, the FFAST database also provides only the mass attenuation coefficient of the element or compound of interest. Furthermore, the Phy-X tool provides a choice to compute mass attenuation coefficient along with 17 more shielding parameters.

The XCOM photon attenuation database tool allows the user to choose the chemical composition (element, compound and mixture) of interest and provides a wide range of gamma photon attenuation data in the energy range of 1 keV and 100 GeV. The tool provides the mass attenuation coefficient values, comprising photon matter interaction phenomena such as photoelectric absorption, scattering (incoherent and coherent) and pair production (nuclear and electronic fields). However, the number of data points obtained from one composite to another are different. For instance, the data points obtained for PVA/Bi, PVA/W and lead were 103, 104 and 102, respectively [17].

The FFAST database restricts the user from working with pure elements or compounds and computes the MAC values from 0.001 keV to 433 keV gamma photons. Similar to the XCOM database, the data points obtained for Pb, W, Bi and BaSO4 were 775, 911, 772 and 262 respectively [18]. The Phy-X tool allows users to choose the desired chemical composition and provides multiple ways to work with desired energies. The user can work with a standard grid with an energy range of 1 keV–100 GeV or opt for selective energy ranges. Unlike XCOM, the Phy-X tool provides directly computed data of 17 shielding parameters and the mass attenuation coefficient values [19].

The XMuDat photon attenuation database is also a user-friendly tool. It allows the user to work with the desired energy range between 1 keV and 50 MeV and simultaneously compute for six different composites of interest. Unlike XCOM and Phy-X, this tool does not allow users to work with their choice of interest and restricts them to work with the elements/compounds/polymers provided within the XMuDat library. However, this tool provides fifty thousand data points, making it unique and helping to identify any minor deviation in the trend [20].

The recently developed PAGEX and MIKE tools import the mass attenuation coefficient database from NIST XCOM [1,2]. Prabhu et al. and K·I.Hussein et al. have conducted studies by comparing the results of these tools to the existing database, but it's unclear which tool is best. While developing a computational software tool to analyze how X-ray and gamma-ray photons interact with matter and their attenuation properties, it's crucial to predict the mass attenuation coefficient. Therefore, a comparative study of the mass attenuation coefficient values would be sufficient to compare these tools. NIST: FFAST, NIST: XCOM, Phy-X and XMuDat tools independently predict mass attenuation coefficient values and are widely used by researchers worldwide. Though, there are some studies reported on usage of various gamma attenuation tools to investigate the gamma shielding ability of different materials, none of the researchers have reported the best tool for the said purpose. Hence, in the present study, the authors have attempted to compare (pros and cons) the various tools by conducting a direct comparative study of the data obtained using these tools and to decide the more appropriate and precise tool.

2. Materials and methods

To mimic the practical scenario of a composite matrix, polyvinyl alcohol (PVA) has been chosen as the base matrix, with tungsten and bismuth as fillers. Similarly, bismuth (Bi), tungsten (W), Gold (Au), Copper (Cu) and Platinum (Pt) were chosen for the pure elemental case, and for the conventional material case, lead (Pb) and barite ($BaSO_4$) were choen for the comparative study. The mass attenuation coefficient of these materials was computed using the following photon attenuation tools and analysed without further modification. Similarly, experimental results of Au, Cu and Pt reported by Ivor Backhurst have been used for analysis without any further modification [21].

1. XMuDat Photon attenuation data version 1.0.1
2. Web version of the NIST XCOM: photon cross sections database
3. Web version of the Phy-X Photon shielding and dosimetry
4. Web version of the NIST FFAST X-Ray Form Factor, Attenuation and Scattering Tables

3. Results and discussion

The mass attenuation coefficient (MAC) of the PVA based W and Bi filled composites and pure materials such as Au, Cu, Pt, Bi, W, Pb and barite ($BaSO_4$) for gamma rays of energy range of 1 keV–50 MeV were computed using Phy-X, XCOM, FFAST and XMuDat Photon attenuation databases. In each combination of composites, Bi & W filler concentrations were varied and analysed for 40 & 70 wt% in PVA/Bi and PVA/W composites respectively.

Fig. 1 describes the variation of MAC values obtained from the mentioned tools for PVA/Bi and PVA/W composites. Beyond 100 keV gamma energy, there is no significant difference in the data obtained from the mentioned tools. Similarly, From Fig. 2, even in the pure elemental and conventional material case, it can be noticed that there is not much difference in MAC values obtained from these tools. From Table 1 at 100 keV, the results show that the MAC value obtained from these mentioned tools of the materials listed above has a slight variation at the fourth decimal point between one another. This result confirms that all the mentioned tools provide almost the same MAC values. However, Figs. 1 and 2 show that the values differ at the absorption edges. Thus, MAC values at the absorption edge energies significantly test the accuracy of the tools. In a comparative study of the dataset obtained from these tools, the MAC values at the absorption energies play a vital role.

Fig. 1 (a) shows the XCOM data of MAC values of the mentioned composites and conventional material lead. It can be seen that the MAC values obtained from the XCOM database possess two values at the K, L and M absorption edge energies, which appears as an anomaly. Practically speaking, K absorption edge is where there is complete absorption of photon energy by K shell electron and similarly L and M absorption edges. Hence, the material should possess one value of MAC at a particular absorption edge. Careful data analysis noticed that the initial value at the absorption energy must be skipped off among the dual MAC

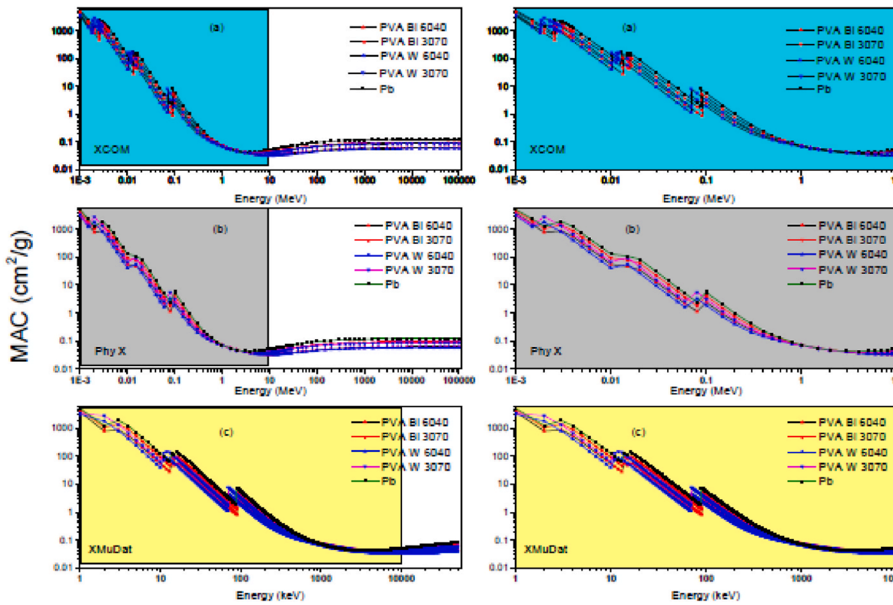

Fig. 1. Mass Attenuation Coefficients of PVA/Bi, PVA/W composites and Lead.

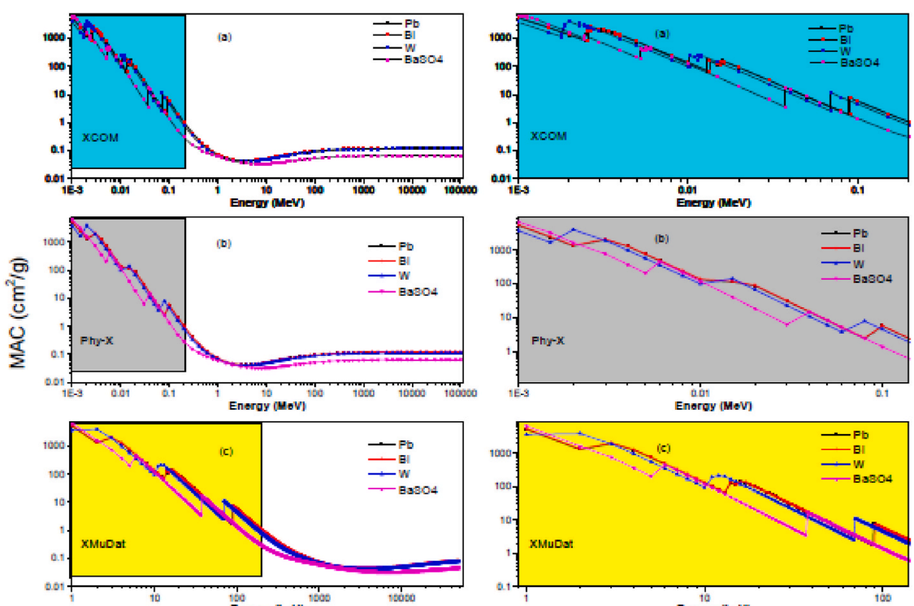

Fig. 2. Mass attenuation coefficients of lead, bismuth, tungsten & barite.

values. However, the tool retains it along with the peak absorption MAC value. This issue was observed as a technical error that could have appeared at the tool development stage. However, this ambiguity in the dataset misleads the users.

Similarly, Fig. 1 (b) shows that the Phy-X tool lacks in providing the sharp absorption edges precisely due to fewer data points in the energy range 1 keV–100 GeV. Furthermore, Fig. 1 (c) represents the variation of MAC values obtained from XMuDat. A large number of data points helps users to identify sharp absorption edges. Unlike XCOM, in this database, ambiguous data points were not found in the given energy range, making this tool more reliable.

To confirm these results, study has been extended to pure and conventional materials such as tungsten, bismuth, lead and barite ($BaSO_4$). Fig. 2 represents the variation of MAC values of these materials with respect to energy obtained from these databases. In which, it can be noticed that the FFAST tool provides much more detailed absorption edge values along with fine structure of X-rays without any ambiguous values at the edges. However, the tool does not compute MAC values of composites and also do not generate the data beyond 433 keV. Here also, a similar lack of data points was observed in Phy-X data and ambiguous two values of MAC were observed at absorption edges in XCOM data. Furthermore, Fig. 3 shows the superimposition of the variations of MAC values of the pure and conventional materials obtained from the above mentioned tools. Variations of MAC values of lead, bismuth, tungsten and barite ($BaSO_4$) also highlight the same result. These results suggest that the XMuDat tool is reliable when compared to other three.

To ascertain these observations, studies on absorption edges were explored. The study of absorption edges provides insight into the behavior of materials, making it a fascinating area of study. Synchrotron Radiation (SR) has made absorption edge studies even more important. Niranjana et al. have attempted to explore K shell parameters of lanthanide elements using bremsstrahlung radiation. They found that

Table 1
Mass attenuation coefficient values of different materials for gamma rays of 100 keV energy using XCOM, Phy-X, FFast and XMuDat tools.

Sl. No.	Material	XCOM	Phy-X	XMuDat	FFAST
1	PVA/Bi 60/40	2.3940	2.3945		2.3870 [a]
2	PVA/Bi 30/70	4.0660	4.0660		4.0530 [a]
3	PVA/W 60/40	1.8740	1.8743		1.8690 [a]
4	PVA/W 30/70	3.1560	3.1556		3.1470 [a]
5	Bi	5.7370	5.7375	5.7190	5.6917[b]
6	W	4.4370	4.4369	4.4240	4.4076[b]
7	Pb	5.5490	5.5491	5.5400	5.5237[b]
8	$BaSO_4$	1.3620	1.3621	1.3700	1.3489[b]

[a] Database do not support to compute the composition.
[b] Mass attenuation co-efficient values at 99.75239 keV.

the experimental and FFAST data curves showed a distinguishable energy gap between points below and above the K edge. However, the fitted curve showed two MAC values at the edge [22]. Fukumachi et al. tried to measure the integrated intensity across the absorption edge of Ga using synchrotron radiation. The experimental data showed a drastic jump in MAC values, which changed as the incident wavelength of the photon changed [23]. Gao et al. noted that for Ge at the K edge, the jump in fano factor is 0.014. This change was observed in the y-axis (fano factor) value which was obtained from the graph of fano factor vs. incident energy. The plot showed a jump in MAC value for two different energies, but not for a single energy [24]. Kulipanov et al. observed a jump in mass attenuation coefficient at the K edge. They noted that “the intensity of the transmitted radiation decreases drastically due to the jump-like change of MAC at the absorption edge if the wavelength is switched on from point A to point B. During the wavelength change from point A to point B, the change of X-ray absorption in the remaining chemical components of the body is insignificant” [25].

Experimental results reported in the literature have been considered and compared with the results obtained from the XMudat, XCOM, Phy-X and FFAST tools and the same are presented in Figs. 4 and 5. Fig. 4 presents the MAC values-both experimental and theoretical values computed using FFAST and least squares fit method for Tb. It is evident that, the computed values are found to be in good agreement with the experimental values. Furthermore no two values of MAC are observed at the absorption edge.

Finally, the experimental data of X-ray interactions with gold, copper and platinum provided by Ivor Blackhurst were plotted without any modification. After examining Fig. 5 and Table 2, it is clear that the MAC values calculated for Au, Cu, and Pt using Phy-X/PSD, XMuDat, FFAST, and experimental data do not have two values at any of the absorption edges. This is in contrast to data from the XCOM database, which does have two values at absorption edges. Additionally, Table 2 shows that XMuDat has relatively a lower percentage of error compared to the other tools mentioned. From Figs. 4 and 5 and Table 2 it is very clear that, there are no two values of μ/ρ (MAC) for a single energy. From these observations, it is clear that MAC values jump drastically at the absorption edge and found to exhibit a single peak value of μ/ρ (evidenced from XMuDAT, PhyX and FFast tools) for a given energy/wavelength as expected to be. Further, upon comparison among these three, owing to

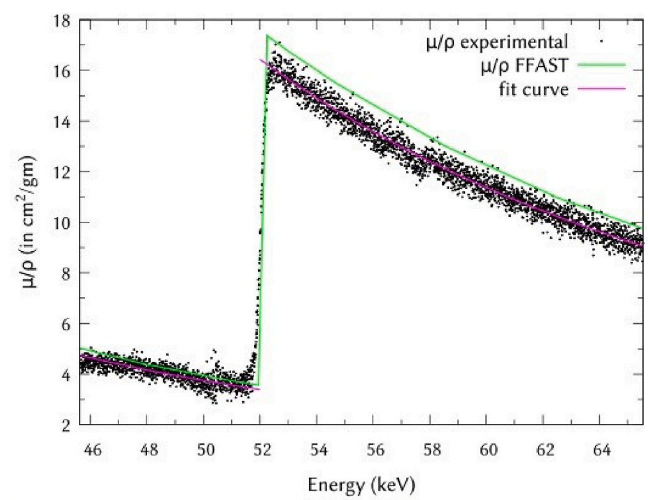

Fig. 4. Plot of MAC as a function of energy for Tb along with least squares fit curves and the theoretical FFAST (Chantler et al., 2005).

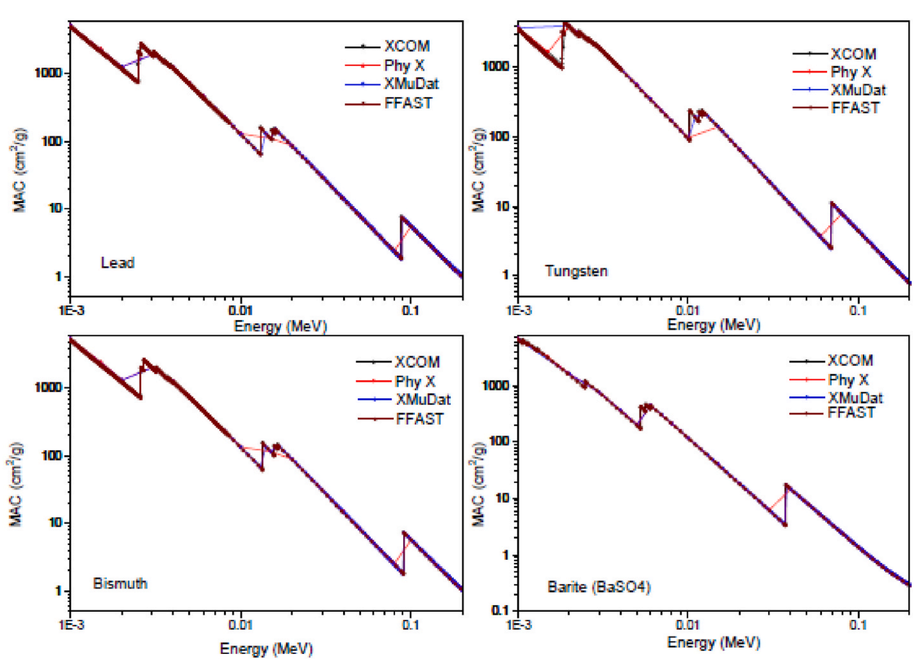

Fig. 3. Mass Attenuation Coefficients of different materials evaluated using different computational software tools below 100 keV photon energy.

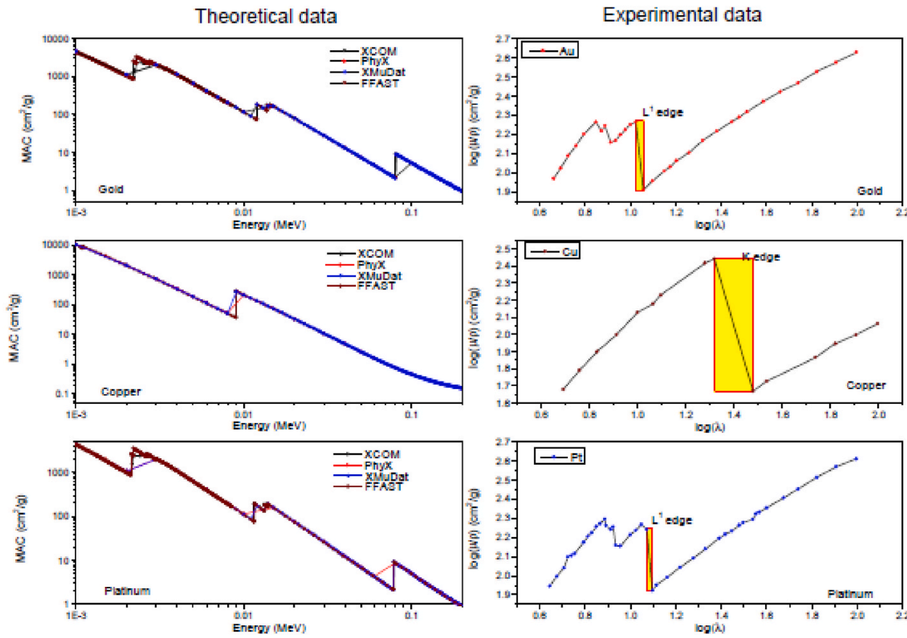

Fig. 5. Mass Attenuation Coefficients of Gold, Copper and Platinum computed using XCOM, Phy-X, XMuDat and FFAST database and obtained experimentally from Ivor backhurst [21]. (For interpretation of the references to colour in this figure legend, the reader is referred to the Web version of this article.)

Table 2
Mass attenuation coefficient values of Gold, Copper and Platinum computed using XCOM, Phy-X and XMuDat tools and obtained from an experimental study [21].

Edge	Experimental (cm^2/g)	XCOM (cm^2/g)	Phy-X (cm^2/g)	XMuDat (cm^2/g)	FFAST (cm^2/g)	XCOM (cm^2/g)	Phy-X (cm^2/g)	XMuDat (cm^2/g)	FFAST (cm^2/g)
						% error			
		MAC values of Au							
L_b^1	81.10	75.83	118.13	90.14	72.79	6.49	45.67	11.15	10.24
L_a^1	184.93	187.0	163.73	181.30	183.24	1.12	11.46	1.96	0.91
		MAC values of Pt							
L_b^1	83.75	78.45	113.23	86.32	75.28	6.33	35.20	3.07	10.12
L_a^1	174.58	194.60	157.76	174.40	190.52	11.47	9.64	0.10	9.13
		MAC values of Cu							
K_b	46.77	38.29	52.55	51.80	37.47	18.14	12.35	10.75	19.89
K_a	275.42	278.30	275.98	275.80	284.68	1.04	0.20	0.14	3.36

Note: Where L_b^1 is the below the edge of L^1 absorption edge and L_a^1 is the above the edge L^1 absorption edge. Similarly, K_b and K_a are below and above the K absorption edges.

its relatively a lower percentage of error, the XMuDat can be considered as a best software tool to evaluate the gamma shielding parameters of the various materials.

4. Summary & conclusions

An attempt was made to compare the reliability of the most trusted tools, such as XCOM, FFAST, Phy-X and XMuDat photon attenuation databases. The MAC values were computed using these tools for PVA/Bi, PVA/W, Pb, Bi, W and barite ($BaSO_4$). The data obtained were plotted without further modification and analysed. A careful analysis of the data revealed that all the mentioned tools provide similar MAC values except at the absorption edge energies. In the case of XCOM, the number of data points obtained for element-to-element and composite-to-composite is different. Also noticed is that this tool makes two MAC values at the absorption edges resulting in ambiguity in measuring MAC values. Similarly, the number of data points obtained from NIST:FFAST tool also varies from sample to sample and can be used only for pure elemental and compound cases. Thus it cannot be used for composite materials and the energy range is limited to 433 keV. The Phy-X tool needs to be figured out in yielding the precise absorption edges as this provides fewer data points in the energy range of 1 keV–100 GeV. On the other hand, the XMuDat provides fifty thousand data points for each mentioned material's MAC values, which helps to identify sharp absorption edges and any minor deviation in the trend. The study also recommends that the XCOM: NIST team would be required to update the web version of XCOM and update the MAC values provided at the absorption edges. Therefore, the XMuDat tool is much more reliable than the other three tools.

CRediT authorship contribution statement

S. Arun Kumar: Methodology, Formal analysis, Writing – original draft. **S.K. Shahsi Kumar:** Experimentation, computational work. **M.R. Ambika:** Conceptualization, Writing – review & editing. **M.B. Karthik Kumar:** Methodology. **N. Nagaiah:** Conceptualization, Writing – review & editing. **Mayeen Uddin Khandaker:** Formal analysis.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

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