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Phy-X / PSD: Development of a user friendly online software for calculation of parameters relevant to radiation shielding and dosimetry

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ABSTRACT

A user friendly online **P**hoton **S**hielding and **D**osimetry (PSD) software available at https://phy-x.net/PSD has been developed for calculation of parameters relevant to shielding and dosimetry. These parameters include linear and mass attenuation coefficients (LAC, MAC), half and tenth value layers (HVL, TVL), mean free path (MFP), effective atomic number and electron density (Z_{eff}, N_{eff}), effective conductivity (C_{eff}) energy absorption and exposure buildup factors (EABF, EBF). The software can generate data on shielding parameters in the continuous energy region (1 keV-100 GeV). Also, some well-known radioactive sources (^{22}Na, ^{55}Fe, ^{60}Co, ^{109}Cd, ^{131}I, ^{133}Ba, ^{137}Cs, ^{152}Eu and ^{241}Am) along with their energies and some characteristic (K-shell) X-ray energies of Cu, Rb, Mo, Ag, Ba and Tb elements are available in the software and can be selected by the user. Thus, one can obtain the shielding parameters at photon energies available for the predefined energies. Moreover, another parameter relevant to shielding i.e. the fast neutron removal cross section (FNRCS) can be calculated for a compound or a mixture using this software. The software is freely available online after having registered to the Phy-X platform.

1. Introduction

Radiation leakage can create serious effects on living organisms (Møller and Mousseau, 2013). Due to wide applications of the radiation in human daily activities, safety demand is increasing for proper radiation shielding day by day. For this reason, researchers are trying to obtain new shielding materials for high energetic electromagnetic radiation such as X- and gamma rays which have been used in many different areas including radiology (Mettler Jr et al., 2008), elemental analysis (Gürol et al., 2016; Kanngießer et al., 2003; Marguí et al., 2005), food irradiation (Farkas, 2006), industry (Hormes and Warner, 2012) and medicine (Reed, 2011) etc.

Lead (Pb) is the well-known element used for the radiation shielding applications. However, due to its some limited characteristic properties such as low melting point (327.5 °C), poor mechanical strength and toxicity, it is necessary to develop new type of protective materials, which do not contain lead. For this purpose, it is important to design new shielding materials having high density, good mechanical strength, low chemical abrasion, high transparency, high melting temperature and low cost. In literature, a great number of studies have been carried out to produce and develop shielding materials having the aforementioned tribological properties. Recently, these studies were mainly focused on enhancing the radiation shielding properties of the materials such as alloys (Akkurt, 2009; Alim et al., 2019a, 2019b; Aygün et al., 2019; Buyukyildiz, 2016; Han et al., 2012; Han and Demir, 2009b, 2010; Kaewkhao et al., 2008; Singh and Badiger, 2013, 2014a), concretes (Akkurt et al., 2005, 2006; Bashter, 1997; El-Khayatt, 2010; Singh and Badiger, 2014b), glasses (Ersundu et al., 2018; Issa et al., 2018; Kaewkhao et al., 2010; Kumar et al., 2018, 2019; Kurudirek et al., 2018; Limkitjaroenporn et al., 2011; Sayyed, 2016; Sayyed and Elhouichet, 2017; Singh et al., 2003, 2008a, 2008b), polymers (Manjunatha, 2017; Midgley, 2005; Sathiyaraj et al., 2017), compounds (Han et al., 2015; Icelli et al., 2013; McCaffrey et al., 2012) and soils (Appoloni and Rios, 1994; Sayyed et al., 2019). As a result of our search in the Web of Science database by using only the keyword “Radiation Shielding” a number of around 1950 articles appeared between 2008 and 2018. Furthermore, it is clear that the number of published articles and associated citations in this area will increase with the use of

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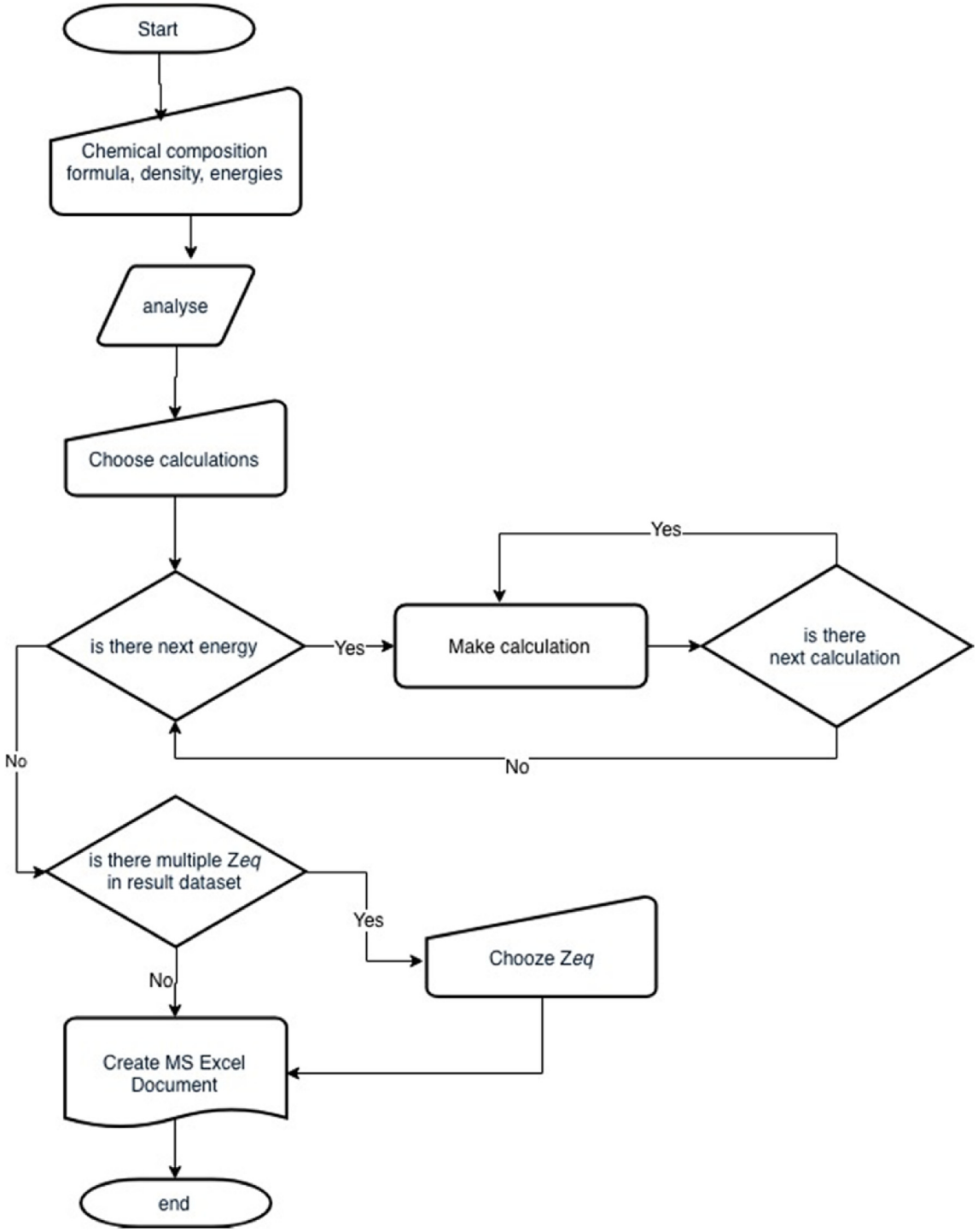

Fig. 1. Flow chart of the PSD online software.

different keywords such as effective atomic number, radiation dosimetry, X- and gamma rays and radiation protection etc.

In the light of the distribution of studies between 2008 and 2018, it is observed that there has been a tremendous interest in studies involving photon attenuation parameters in the past few decades. This situation shows the importance of studies in the field of radiation shielding. In the majority of these studies, radiation attenuation parameters such as linear attenuation coefficient (LAC), half and tenth value layers (HVL and TVL), mean free path (MFP), effective atomic number (Z_{eff}), effective electron number (or effective electron density) (N_{eff}), effective conductivity (C_{eff}) and buildup factors are calculated in order to obtain the best shielding material in a certain or continuous energy region. Due to the large amount of these parameters, it is quite time-consuming to make these calculations correctly. Calculation of these parameters for composite materials especially in continuous energy region requires compiling enormous amount of data and manual calculation of these parameters needs a huge effort. Therefore, it is significant and necessary to calculate all these parameters more quickly, practically and accurately in a continuous energy range or at selected energies. From this point of view, Hubbell and Seltzer (1995) reported the MAC for several elements in the energy region of 1 keV–20 MeV because of the fact that the theoretical calculation of all the above-

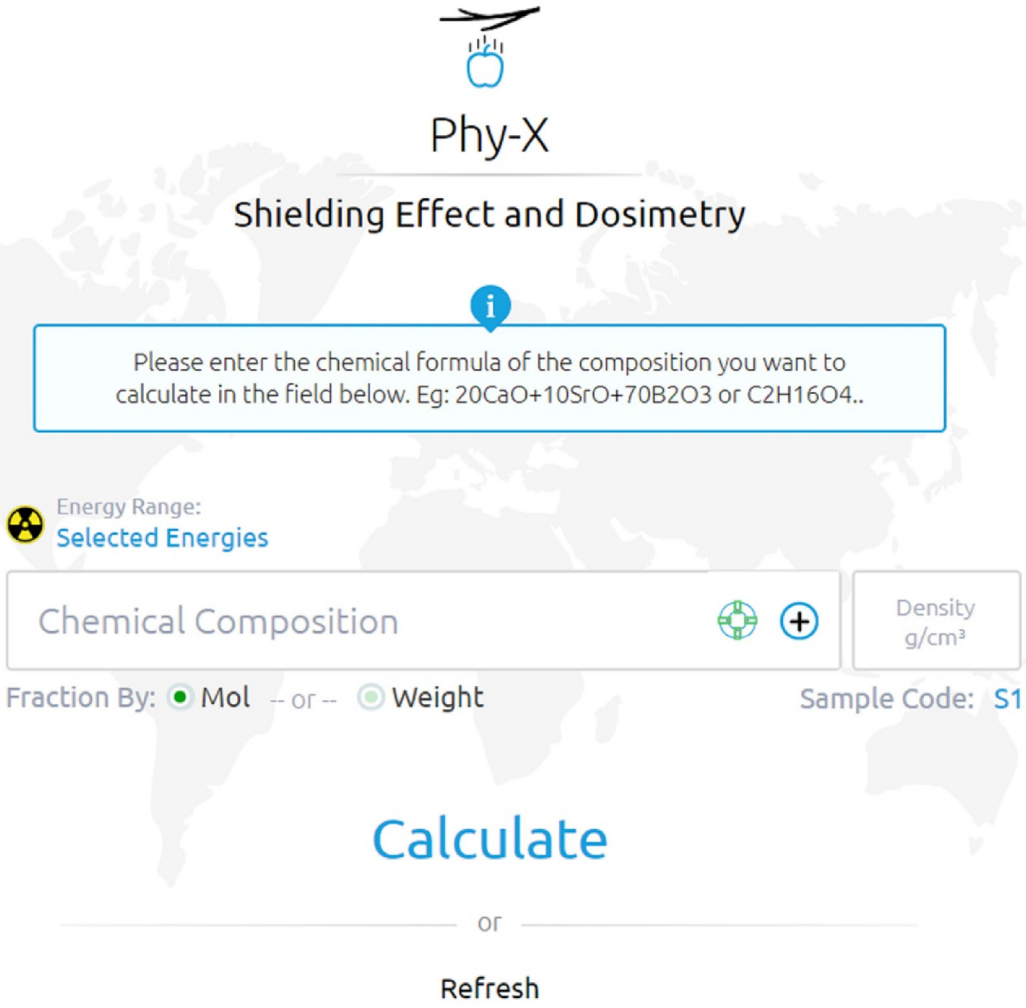

Fig. 2. Main screen of the PSD online software.

mentioned shielding parameters is based on MAC values (Hubbell and Seltzer, 1995). This work was a sequel of their previous work (Hubbell, 1982). The reported values of the uncertainties in estimating MACs were about 1–2% in the region of 5 keV to a few MeV whereas they reach to about 25–50% between 1 keV and 4 keV (Hubbell, 1999). These high uncertainties below 4 keV were adequately addressed and new theoretical results of substantially higher accuracy in near-edge soft X-ray regions were derived (Chantler, 2000).

There are some useful softwares introduced in the literature to meet the above mentioned needs. WinXCOM (Gerward et al., 2001, 2004) (early developed as XCOM (Berger and Hubbell, 1987)) and XMuDat (Nowotny, 1998) have been developed for calculation of MACs for elements, compounds and mixtures in the continuous energy region. More recently, a computer program for the calculation of mass energy-absorption coefficients for body tissues of different weight composition has been developed (Okunade, 2007). Thereafter, different researchers have paid an effort to develop user friendly programs for calculation of another photon interaction parameter namely Z_{eff}, which is related to radiation interaction processes and is relevant for composite media. For example, Auto-Zeff program has been developed which can calculate the Z_{eff} for any materials at different energies (Taylor et al., 2012). The Direct-Z_{eff} software has been developed to give the MAC, the Z_{eff} and the N_{eff} for partial photon interactions i.e., coherent and incoherent scattering, photoelectric absorption and pair production as output data (Un and Caner, 2014). Moreover, the ZXCOM software (originally published as elsewhere (Yalcin et al., 2012) has been developed to generate considerable predications for Z_{eff}, N_{eff}, and the Rayleigh to Compton scattering ratios for different materials under different experimental conditions (Eyecioglu et al., 2016). Recently, Eyecioğlu et al. (2019) developed BXCOM software for the calculation of EBF and EABF parameters for the compounds and mixture (Eyecioğlu et al., 2019). However, to the best of our knowledge a software which can calculate all parameters relevant to shielding and dosimetry as explained early has not become available yet. In this study, the PSD software have been developed which can simultaneously calculate all above mentioned shielding and dosimetric parameters in continuous energy range and at selected energies in a fast and accurate way for an infinite number of different materials.

2. Theory

The MAC is a quantity that describes the interaction probability between gamma photons and the mass per unit area for a certain medium and can be calculated by the well-known Beer–Lambert as follows:

$$I = I_0 e^{-\mu t} \tag{1}$$

$$\mu_m = \left(\frac{\mu}{\rho}\right) = \frac{\ln(I_0/I)}{\rho t} = \frac{\ln(I_0/I)}{t_m} \tag{2}$$

where I_o and I are un-attenuated and attenuated photon intensities, $\mu(\mathrm{cm}^{-1})$ and $\mu_m(\mathrm{cm}^2/\mathrm{g})$ are linear and mass attenuation coefficients, t (cm) and t_m ($\mathrm{g/cm}^2$) are the thickness and sample mass thickness (the mass per unit area), and ρ ($\mathrm{g/cm}^3$) is the density of material.

Table 1
Examples for definition of materials.

Mole Fraction Input Examples (Sum of the coefficients have to be equal to 100)			
	Types of Materials	Contents (Mole amount; mol)	Example Input Type
1	Pure Element	Pb (—)	Pb or 100 Pb
2	Single Compounds	C_2H_5OH (—)	C2H5OH or 100C2H5OH
3	Multi Compound (Total 10 mole Material)	Bi_2O_3 (7.000) SiO_2 (3.000)	70Bi2O3 + 30SiO2
4	Multi Compound (Total 2.3 mole Material)	Bi_2O_3 (0.200) SiO_2 (0.700) PbO (1.400)	8.7Bi2O3 + 30.4SiO2 + 60.9PbO
5	Mixture (example for alloys)	Fe (0.681) Cr (0.221) Al (0.097) Y (0.001) Zr (0.001)	68.1Fe + 22.1Cr + 9.7Al + 0.1Y + 0.1Zr
Weight Fraction Input Examples (Sum of the coefficients have to be equal to 1)			
	Types of Materials	Contents (Weight amount; g)	Example Input Type
1	Pure Element	Pb (—)	1 Pb
2	Single Compounds	C_2H_5OH (—)	1C2H5OH
3	Multi Compound (Total 10 gr Material)	Bi_2O_3 (7.000) SiO_2 (3.000)	0.7Bi2O3 + 0.3SiO2
4	Multi Compound (Total 21 gr Material)	Bi_2O_3 (5.000) SiO_2 (7.000) PbO (9.000)	0.238Bi2O3 + 0.333SiO2 + 0.429PbO
5	Mixture (example for alloys)	Fe (72.800) Cr (22.000) Al (5.000) Y (0.100) Zr (0.100)	0.728Fe + 0.220Cr + 0.050Al + 0.001Y + 0.001Zr

Table 2
The list of the radioactive sources and characteristic X-ray energies used in the software.

Source		Characteristic X-ray energies (MeV)						
		Cu	Rb	Mo	Ag	Ba	Tb	
Kα		0.00804	0.01337	0.01744	0.02210	0.03206	0.04448	
Kβ		0.00891	0.01497	0.01963	0.02490	0.03639	0.05038	
Radioisotope source energies (MeV)								
Co^{60}	Am^{241}	Cs^{137}	Fe^{55}	Ba^{133}	I^{131}	Eu^{152}	Na^{22}	Cd^{109}
0.34714	0.01381	0.28350	0.00589	0.03500	0.36449	0.03950	0.51100	0.02210
0.82610	0.02634	0.66166	0.00590	0.03580	0.63699	0.04012	1.27500	0.02310
1.17323	0.03218		0.00649	0.03082	0.28400	0.04590		0.02500
1.33249	0.03320		0.00654	0.03540	0.08000	0.04704		0.02550
2.50569	0.05954			0.05316	0.72300	0.12178		0.08804
	0.09897			0.04962		0.24470		
	0.10298			0.08100		0.29594		
				0.16061		0.34428		
				0.22340		0.41112		
				0.27640		0.44396		
				0.30285		0.67800		
				0.35602		0.68867		
				0.38385		0.77890		
						0.86737		
						0.96408		
						1.00530		
						1.08590		
						1.08970		
						1.11210		
						1.29910		
						1.40800		
						1.45760		

The μ_m for any sample can be estimated using equation (3) namely (Jackson and Hawkes, 1981):

$$\mu_m = \left(\frac{\mu}{\rho}\right) = \sum_i w_i(\mu/\rho)_i \quad (3)$$

where w_i is the weight fraction of the ith constituent element.

HVL and TVL are the required thicknesses to reduce the radiation intensities by one half and one tenth, respectively. The linear attenuation coefficient (μ) is used to obtain these parameters as follows:

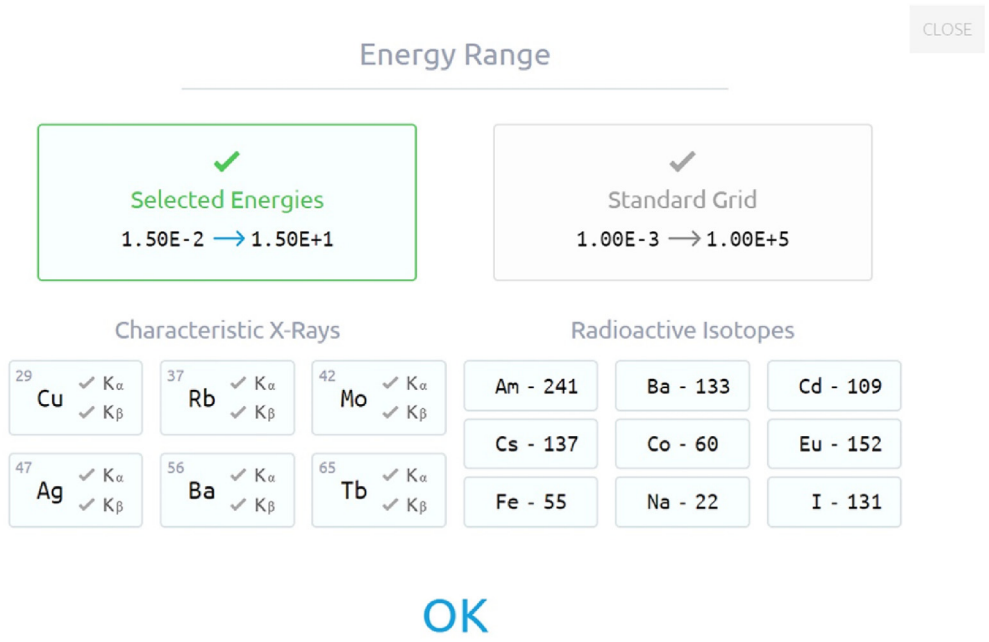

Fig. 3. The energy options that users can select in the PSD online software.

$$HVL = \frac{\ln(2)}{\mu} = \frac{0.693}{\mu} \; and \; TVL = \frac{\ln(10)}{\mu} = \frac{2.302}{\mu} \tag{4}$$

The MFP is a term that describes the average distance between two interactions of photons and can be evaluated from μ (cm^{-1}) using the following formula:

$$MFP = \frac{\int_0^\infty te^{(-\mu t)}dt}{\int_0^\infty e^{(-\mu t)}dt} = \frac{1}{\mu} \tag{5}$$

The total atomic cross-sections (σ_a; cm^2/g) for any sample can be calculated from the mass attenuation coefficients utilizing the next equation:

$$\sigma_a = \frac{N\mu_m}{N_A} \tag{6}$$

In the previous equation, N_A is Avogadro constant.

The total electronic cross-sections (σ_e; cm^2/g)is given by the following formula (Han and Demir, 2009a):

$$\sigma_e = \frac{1}{N_A}\left(\sum_i \frac{f_i A_i}{Z_i}(\mu_m)_i\right) = \frac{\sigma_a}{Z_{eff}} \tag{7}$$

where Z_i, f_i, $(\mu_m)_i$ andA_i are the atomic number, mole fraction, mass attenuation coefficient and atomic weight of the i*th* constituent element, respectively. Z_{eff} represents the effective atomic number of the material. From the parameters given in Equation (6) and equation (7), we can evaluate Z_{eff} using the next relation:

$$Z_{eff} = \frac{\sigma_a}{\sigma_e} \tag{8}$$

Moreover, (N_{eff}; $electrons/g$) is given by the next formula (Han and Demir, 2009b):

$$N_{eff} = \frac{N_A}{N} Z_{eff} \sum_i n_i = \frac{\mu_m}{\sigma_e} \tag{9}$$

where $\sum n_i$ is the total number of elements in the material.

Effective Conductivity (C_{eff}; S/m)of materials is directly proportional to the$N_{eff}$and given by following equation (Manjunatha, 2017):

$$C_{eff} = \left(\frac{N_{eff}\rho e^2 \tau}{m_e}\right)10^3 \tag{10}$$

where e (C) and $m_e(kg)$are charge and mass of electron, respectively, and N_{eff} should be considered electrons/kg, $\tau(s)$is the average life time (relaxation time) of the electron at the Fermi Surface and is defined by the following formula (Devillers, 1984):

$$\tau = \frac{\hbar}{k_B T} = \frac{h}{2\pi k_B T} \tag{11}$$

where h $(J.s)$, k_B (J/K) and T (K) are the Planck constant, Boltzman constant and temperature of the environment.

If the geometry used in the absorption experiments is broad-beam geometry, the Beer-Lambert law given in Eq. (1) would be no longer valid and it turns out to be $I = BI_0e^{-\mu x}$. Here, B is a correction term and is called as "photon build-up factor". Build-up factor is divided to two types namely exposure buildup factor (EBF) and energy absorption buildup factor (EABF). The EBF and EABF calculation procedures are the same except for the coefficients used available in ANSI database. The Geometric Progression (G-P) fitting is a method used to calculate the buildup factors. For EBF and EABF calculations, the steps are described below:

In the first step, the ratio of Compton partial mass attenuation coefficient to total mass attenuation coefficient (R; $(\mu_m)_{Compton}/(\mu_m)_{Total}$)must be defined for the material at certain energy. The R value obtained for the material must be between the $(\mu_m)_{Compton}/(\mu_m)_{Total}$ values calculated for the two adjacent elements. In the previous equation, the R_1 and R_2 values denotes the $(\mu_m)_{Compton}/(\mu_m)_{Total}$ ratios of these two adjacent elements which have Z_1 and Z_2 atomic numbers.

In the second step, one can calculate the equivalent atomic number (Z_{eq}) using the equation:

$$Z_{eq} = \frac{Z_1(\log R_2 - \log R) + Z_2(\log R - \log R_1)}{\log R_2 - \log R_1} \tag{12}$$

In the third step, the geometric progression (G-P) fitting parameters (a, b, c, d, XK) of the material must be calculated. In order to calculate G-P fitting parameters, a similar logarithmic interpolation procedure is applied as in the case of Zeq. The G-P fitting parameters of the some elements (Z = 4–92) were tabulated in the energy range between 0.015 and 15 MeV (ANSI/ANS-6.4.3 (1991)). Five different G-P fitting parameters can be calculated using the interpolation expression suggested by Harima (1983).

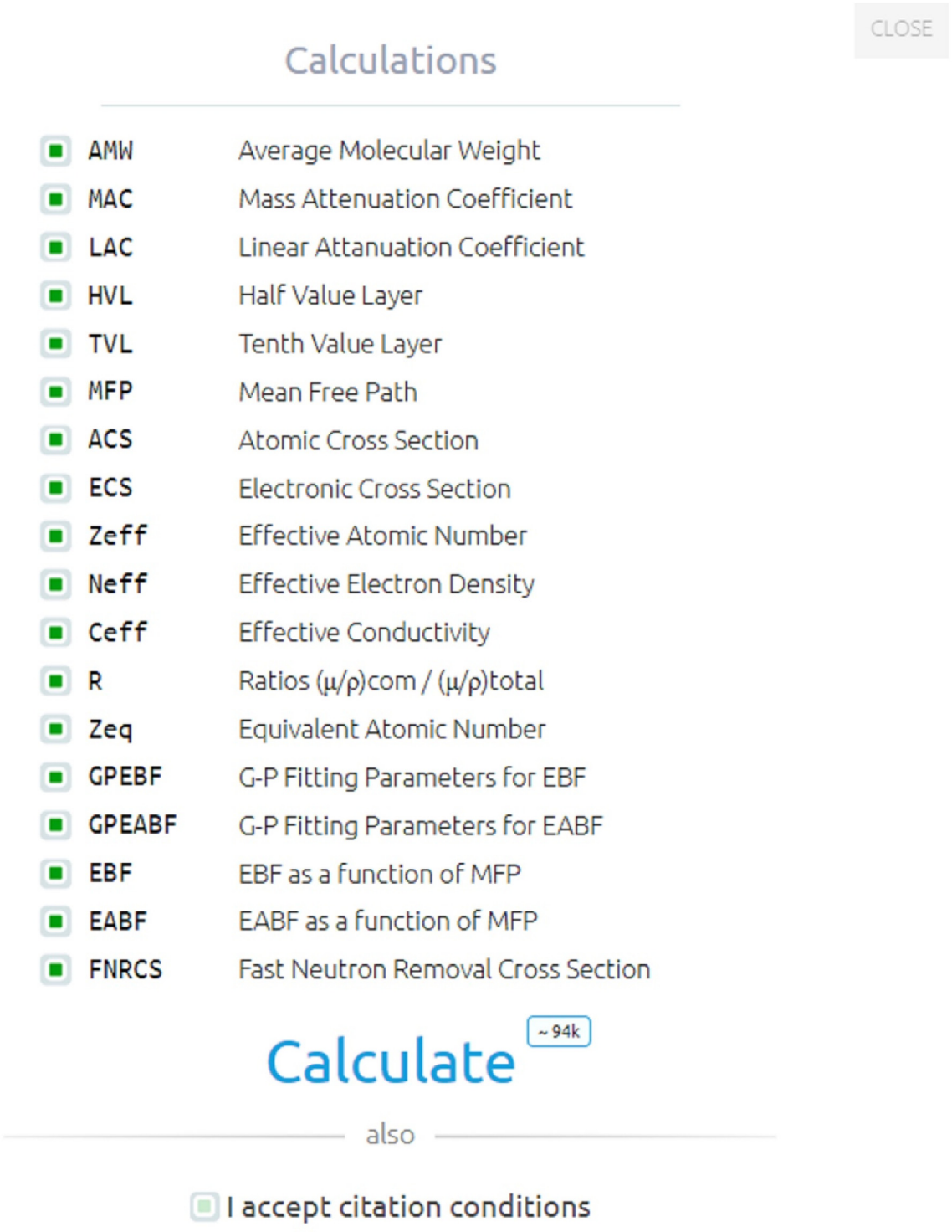

Fig. 4. The selection of calculated parameters which can choosing by users.

$$P = \frac{P_1(\log Z_2 - \log Z_{eq}) + P_2(\log Z_{eq} - \log Z_1)}{\log Z_2 - \log Z_1} \tag{13}$$

where P represents the G-P fitting parameters (a, b, c, d and X_K coefficients) of investigated material. In Eq. (13), P_1 and P_2 are the values of G-P fitting parameters (obtained from ANSI database) corresponding to the Z_1 and Z_2 atomic numbers at a certain energy, respectively.

In the last step, one can calculate the build-up factor (EBF and/or EABF) with the help of the G-P fitting parameters obtained from Eq. (13) using the equations:

$$B(E,X) = \begin{cases} 1 + \frac{(b-1)(K^X-1)}{K-1} & for\ K \neq 1 \\ 1 + (b-1)X & for\ K = 1 \end{cases} \tag{14}$$

where E and X denotes primary photon energy and penetration depth, respectively. The X values vary from 0.5 to 40 MFP and are generally calculated for 16 different values.

The function $K(E, X)$can be calculated using the following equation:

Table 3
The selectable parameters and parameters required for their calculation.

Parameters number	Parameters	Abbreviation of parameters	Required parameters
1	Average Molecular Weight	AMW	Definition of material (see section 3.1)
2	Mass Attenuation Coefficient	MAC	Energy, Definition of material
3	Linear Attenuation Coefficient	LAC	Energy, MAC, Density of material (g/cm^3)
4	Half Value Layer	HVL	Energy, MAC, Density of material (g/cm^3)
5	Tenth Value Layer	TVL	Energy, MAC, Density of material (g/cm^3)
6	Mean Free Path	MFP	Energy, MAC, Density of material (g/cm^3)
7	Atomic Cross Section	ACS	Energy, Definition of material
8	Electronic Cross Section	ECS	Energy, Definition of material
9	Effective Atomic Number	Z_{eff}	Energy, Definition of material
10	Effective Electron Density	N_{eff}	Energy, Z_{eff}, Definition of material
11	Effective Conductivity	C_{eff}	Energy, N_{eff}, Z_{eff}, Definition of material, Density of material (g/cm^3)
12	Ratios (μ/ρ)Com/(μ/ρ)total	R	Energy, Definition of material
13	Equivalent Atomic Number	Z_{eq}	Energy (only 0.015–15 MeV), R, Closest Elements (see Fig. 7)
14	G-P Fitting Parameters for EBF	GPEBF	Energy (only 0.015–15 MeV), R, Z_{eq}
15	G-P Fitting Parameters for EABF	GPEABF	Energy (only 0.015–15 MeV), R, Z_{eq}
16	EBF as a function of MFP	EBF	Energy (only 0.015–15 MeV), R, Z_{eq}, GPEBF
17	EABF as a function of MFP	EABF	Energy (only 0.015–15 MeV), R, Z_{eq}, GPEABF
18	Fast Neutron Removal Cross Section	FNRCS	Density, Definition of material

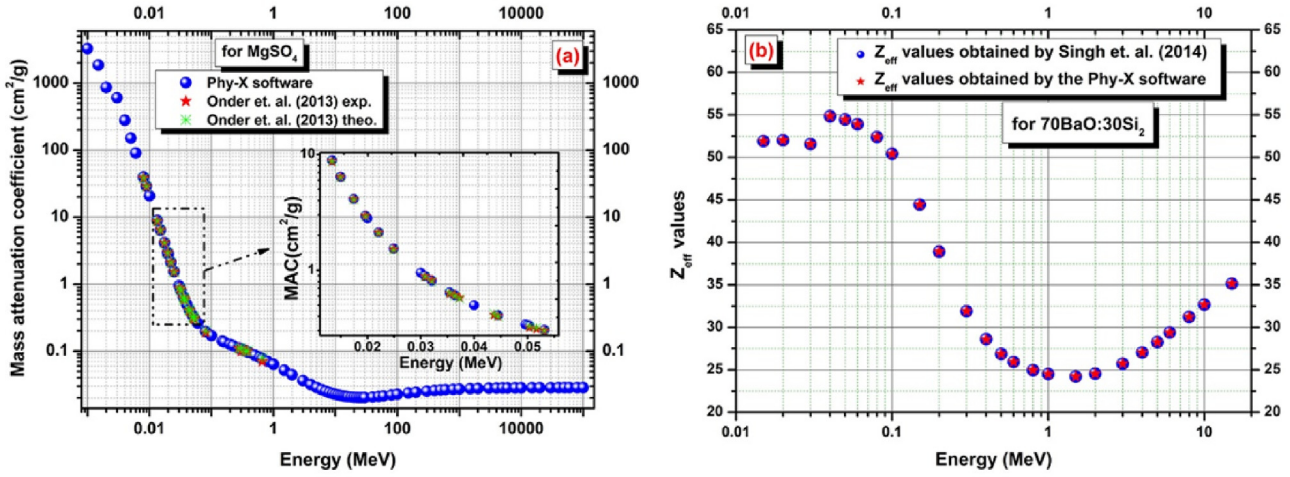

Fig. 5. (a) Comparison of experimental and theoretically $MgSO_4$ samples with PSD software results **(b)** Comparison of Z_{eff} values obtained by Singh et al. (2014) with the results obtained from the PSD online software.

$$K(E,X) = cX^a + d\frac{\tanh((X/X_K) - 2) - \tanh(-2)}{1 - \tanh(-2)} \quad for\ penetration\ depth\ (X) \le 40\ mfp \tag{15}$$

Combination of $K(E,X)$ with X, perform the photon dose multiplication and determine the shape of the spectrum.

It is well known that since the neutrons are particles with no charge, they can interact with a medium through different mechanisms. The main mechanisms are elastic and inelastic scattering, nuclear fission, nuclear spallation and neutron capture. In order to calculate the potentiality of any sample to attenuate the neutron, the fast neutron removal cross section (FNRCS) (Σ_R) is considered a common parameter used in this regard. The following relation is used for the calculation of $\sum R$:

$$\sum_R = \sum_i \rho_i (\Sigma_R/\rho)_i \tag{16}$$

where, ρ_i and $(\Sigma_R/\rho)_i$ are the partial density and mass removal cross-section of the ith constituent, respectively (Wood, 1982). The mass removal cross-section values for the elements were adopted from Kaplan and Chilton (Chilton et al., 1984; Kaplan, 1989).

3. The Phy-X/PSD online software

The Phy-X/PSD online software is running on remote server that has Intel(R) Core(TM) i7-2600 CPU @ 3.40 GHz CPU with 1 GB installed memory and operating system is Ubuntu 14.04.3 LTS. The application language is NodeJS v8.4.0 serving with Nginx 1.15.8. Security between client's browser and server is being established with 256 Bit Positive SSL. In order to use the PSD software, the users must have access to the web page of https://phy-x.net/PSD. The flow chart and the main screen interface of the PSD online software are shown in Figs. 1 and 2, respectively. Users must register with the Phy-X platform in order to calculate the radiation shielding parameters of any material. The registration process can be completed by verification using only academic e-mail addresses. There are three steps which are necessary for calculation in the software and are listed as follows:

3.1. Definition of materials

The first step is to define the composition of the material to be used in calculations accurately. In the software, the material composition can be entered in two different ways such as mole fraction and weight fraction. After the selection of mole or weight fraction in the software, the users make sure that the sum of mole fractions or weight fractions is equal to 100 or 1, and if necessary users must normalize them before

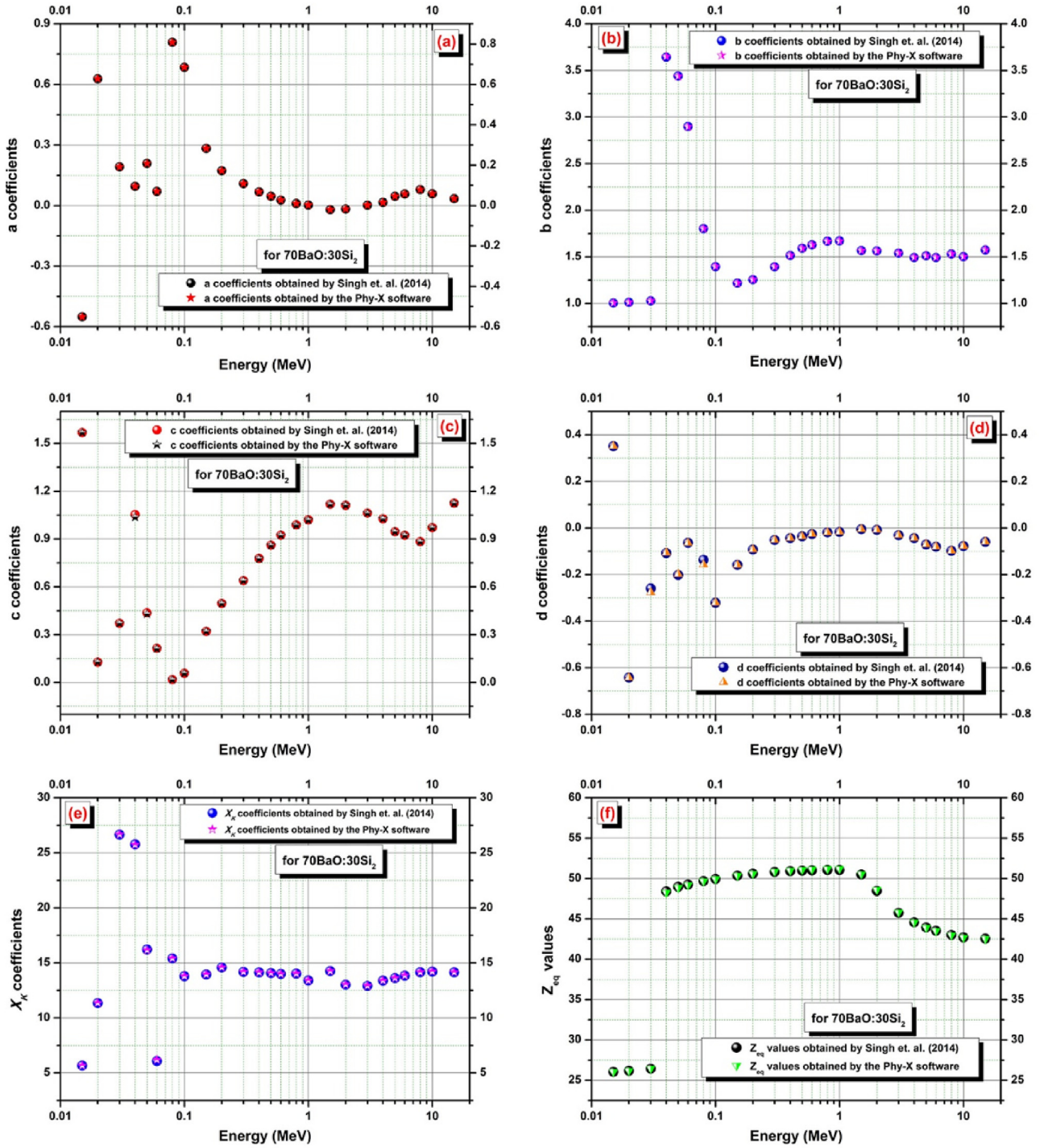

Fig. 6. Comparison of G-P fitting parameters (a, b, c, d and X_K) and Z_{eq} values repoted by Singh et al. (2014) with the results obtained from the PSD online software.

entering fractions to the program. The examples describing this situation are given in Table 1. In the software there is no any limitation for the addition of compound or elements. In order to add new content to the materials, the symbol of plus (+) must be used between the contents such as $70Bi_2O3+30SiO_2$ and 68.1Fe + 22.1Cr + 9.7Al + 0.1Y + 0.1Zr (see Table 1). The PSD online software can produce data for unlimited number of different materials, which can be added by using + symbol in the main screen of the software, at the same time. Namely, when the user clicks each + sign, a new line is opened up so that the user can enter a new material composition. Additionally, the density (g/cm^3) of the phase state in which the material is used as shielding is required for LAC, HVL, TVL, MFP, C_{eff} and FNRCS parameters, and label of the materials to be calculated must be written to the boxes in the relevant line.

3.2. Selection of energies

Two energy regions have been predefined in the software as 15 keV-15 MeV (relevant to ANSI database and is used in calculation of EABF and EBF) and 1 keV-100 GeV. Also, some well-known radioactive sources (^{22}Na, ^{55}Fe, ^{60}Co, ^{109}Cd, ^{131}I, ^{133}Ba, ^{137}Cs, ^{152}Eu and ^{241}Am) along with their energies and some characteristic X-ray energies obtained through secondary sources (the K-shell energies of Cu, Rb, Mo, Ag, Ba and Tb elements) are available in the software and can be

Table 4
Comparison of some parameters for 70 BaO:30 SiO2 sample with Phy-X/PSD and the Singh's results.

Energy (MeV)	a coeff.		b coeff.		c coeff.		d coeff.		Xk coeff.		Zeq		Zeff	
	Singh et al.	Phy-X/PSD	Singh et al.	Phy-X/PSD	Singh et al.	Phy-X/PSD	Singh et al.	Phy-X/PSD	Singh et al.	Phy-X/PSD	Singh et al.	Phy-X/PSD	Singh et al.	Phy-X/PSD
1.50E-02	−0.551	−0.551	1.004	1.004	1.568	1.568	0.351	0.351	5.677	5.675	26.040	26.038	51.920	51.911
2.00E-02	0.628	0.628	1.012	1.012	0.128	0.128	−0.642	−0.642	11.354	11.354	26.170	26.166	52.020	52.012
3.00E-02	0.192	0.192	1.027	1.027	0.372	0.372	−0.260	−0.276	26.655	26.661	26.440	26.442	51.570	51.571
4.00E-02	0.095	0.095	3.642	3.649	1.054	1.037	−0.108	−0.106	25.772	25.718	48.410	48.252	54.850	54.845
5.00E-02	0.209	0.209	3.442	3.436	0.437	0.430	−0.202	−0.198	16.224	16.152	48.970	48.847	54.460	54.461
6.00E-02	0.070	0.070	2.899	2.894	0.214	0.212	−0.064	−0.064	6.080	6.189	49.250	49.179	53.910	53.914
8.00E-02	0.809	0.809	1.803	1.802	0.018	0.018	−0.137	−0.157	15.411	15.407	49.680	49.646	52.390	52.395
1.00E-01	0.685	0.685	1.394	1.394	0.058	0.058	−0.321	−0.321	13.790	13.790	49.940	49.929	50.410	50.396
1.50E-01	0.283	0.283	1.218	1.218	0.321	0.321	−0.158	−0.158	13.938	13.939	50.360	50.345	44.440	44.432
2.00E-01	0.173	0.173	1.255	1.255	0.496	0.496	−0.093	−0.093	14.583	14.583	50.590	50.582	38.910	38.925
3.00E-01	0.109	0.109	1.393	1.393	0.639	0.638	−0.052	−0.052	14.182	14.180	50.810	50.842	31.910	31.916
4.00E-01	0.068	0.068	1.515	1.514	0.778	0.777	−0.044	−0.044	14.137	14.137	50.910	50.980	28.610	28.570
5.00E-01	0.046	0.046	1.592	1.590	0.861	0.860	−0.036	−0.036	14.066	14.066	50.980	51.072	26.870	26.874
6.00E-01	0.027	0.027	1.628	1.626	0.924	0.923	−0.026	−0.026	13.988	13.984	51.010	51.129	25.930	25.929
8.00E-01	0.010	0.010	1.668	1.666	0.989	0.987	−0.019	−0.019	14.022	14.013	51.050	51.180	24.960	24.964
1.00E+00	0.003	0.003	1.672	1.670	1.020	1.019	−0.017	−0.017	13.400	13.396	51.050	51.189	24.510	24.508
1.50E+00	−0.020	−0.020	1.568	1.567	1.118	1.118	−0.005	−0.005	14.251	14.245	50.490	50.553	24.210	24.219
2.00E+00	−0.017	−0.017	1.564	1.563	1.111	1.111	−0.008	−0.008	13.014	13.022	48.460	48.601	24.550	24.542
3.00E+00	0.002	0.002	1.540	1.540	1.062	1.062	−0.031	−0.031	12.914	12.915	45.750	45.809	25.720	25.734
4.00E+00	0.016	0.016	1.493	1.493	1.027	1.027	−0.044	−0.044	13.384	13.384	44.570	44.550	27.050	27.038
5.00E+00	0.046	0.046	1.511	1.512	0.946	0.946	−0.071	−0.071	13.616	13.615	43.940	43.883	28.260	28.275
6.00E+00	0.057	0.057	1.493	1.493	0.923	0.923	−0.081	−0.081	13.841	13.840	43.530	43.494	29.390	29.378
8.00E+00	0.079	0.079	1.530	1.530	0.883	0.883	−0.098	−0.098	14.151	14.151	43.010	42.962	31.240	31.235
1.00E+01	0.058	0.058	1.502	1.502	0.972	0.971	−0.078	−0.078	14.207	14.207	42.710	42.672	32.680	32.688
1.50E+01	0.034	0.034	1.574	1.574	1.125	1.124	−0.060	−0.060	14.141	14.142	42.560	42.523	35.150	35.156

Table 5
Absolute deviations of results given in Table 4.

Energy (MeV)	Absolute Deviations (%)						
	a coeff.	b coeff.	c coeff.	d coeff.	X_K coeff.	Z_{eq}	Z_{eff}
1.50E-02	0.000	0.004	0.030	0.011	0.034	0.006	0.017
2.00E-02	0.000	0.017	0.336	0.020	0.004	0.015	0.016
3.00E-02	0.000	0.023	0.086	6.119	0.023	0.009	0.003
4.00E-02	0.000	0.190	1.567	1.676	0.210	0.327	0.009
5.00E-02	0.000	0.163	1.519	1.990	0.443	0.252	0.001
6.00E-02	0.000	0.172	0.860	0.703	1.788	0.144	0.008
8.00E-02	0.000	0.054	1.944	14.460	0.024	0.068	0.010
1.00E-01	0.000	0.005	0.034	0.078	0.002	0.021	0.028
1.50E-01	0.000	0.025	0.087	0.038	0.007	0.030	0.018
2.00E-01	0.000	0.006	0.085	0.097	0.001	0.015	0.039
3.00E-01	0.000	0.026	0.085	0.673	0.012	0.063	0.018
4.00E-01	0.000	0.068	0.143	0.909	0.000	0.137	0.140
5.00E-01	0.000	0.110	0.117	0.583	0.003	0.180	0.015
6.00E-01	0.000	0.117	0.101	0.615	0.027	0.233	0.005
8.00E-01	0.000	0.115	0.159	1.105	0.061	0.254	0.016
1.00E+00	0.000	0.113	0.085	1.647	0.031	0.273	0.008
1.50E+00	0.000	0.044	0.018	0.600	0.045	0.125	0.036
2.00E+00	0.000	0.043	0.008	2.000	0.060	0.290	0.031
3.00E+00	0.000	0.005	0.046	1.000	0.005	0.129	0.056
4.00E+00	0.000	0.011	0.006	1.114	0.003	0.046	0.044
5.00E+00	0.000	0.046	0.024	0.169	0.006	0.129	0.054
6.00E+00	0.000	0.026	0.044	0.593	0.007	0.082	0.041
8.00E+00	0.000	0.014	0.052	0.480	0.002	0.112	0.017
1.00E+01	0.000	0.012	0.083	0.346	0.002	0.090	0.025
1.50E+01	0.000	0.022	0.061	0.550	0.009	0.087	0.017

selected by the user. The list of the source energies used in the software is given in Table 2 and energy options that users can select in the software are shown in Fig. 3.

3.3. Selection of parameters to be calculated

Users can choose which parameter(s) they want to calculate depending on their studies (Fig. 4). After defining the materials as described in section 3.1, the software needs some parameters for the selected calculations. The required parameters for the calculation(s) are listed in Table 3. The MAC values used in these calculations are taken from the NIST (National Institute of Standard and Technology) database (Berger and Hubbell, 1987). The users are free to choose both the energies and the number of parameters to be calculated.

After the steps (described in sections 3.1-3.3) completed successfully, users can save the calculation results in a well-designed MS excel file. An example calculation was done for the compositions of $20WO_3 + xBi_2O_3 + (80\text{-}x)TeO_2$ (x = 10, 15, 20 and 25 mol%) (Gaikwad et al., 2019) (for four samples). The screenshot of the data input page of the compositions and obtained results (MS excel file) are given in the supplementary material file. As can be seen from this file, all the calculation results obtained for the different material compositions are saved in the same excel file. Additionally, the most basic of radiation shielding parameters such as MAC, LAC, HVL, MFP, ACS, ECS, Z_{eff}, N_{eff}, C_{eff}, R and Z_{eq} are given comparatively so that the users can evaluate the analysis results more easily.

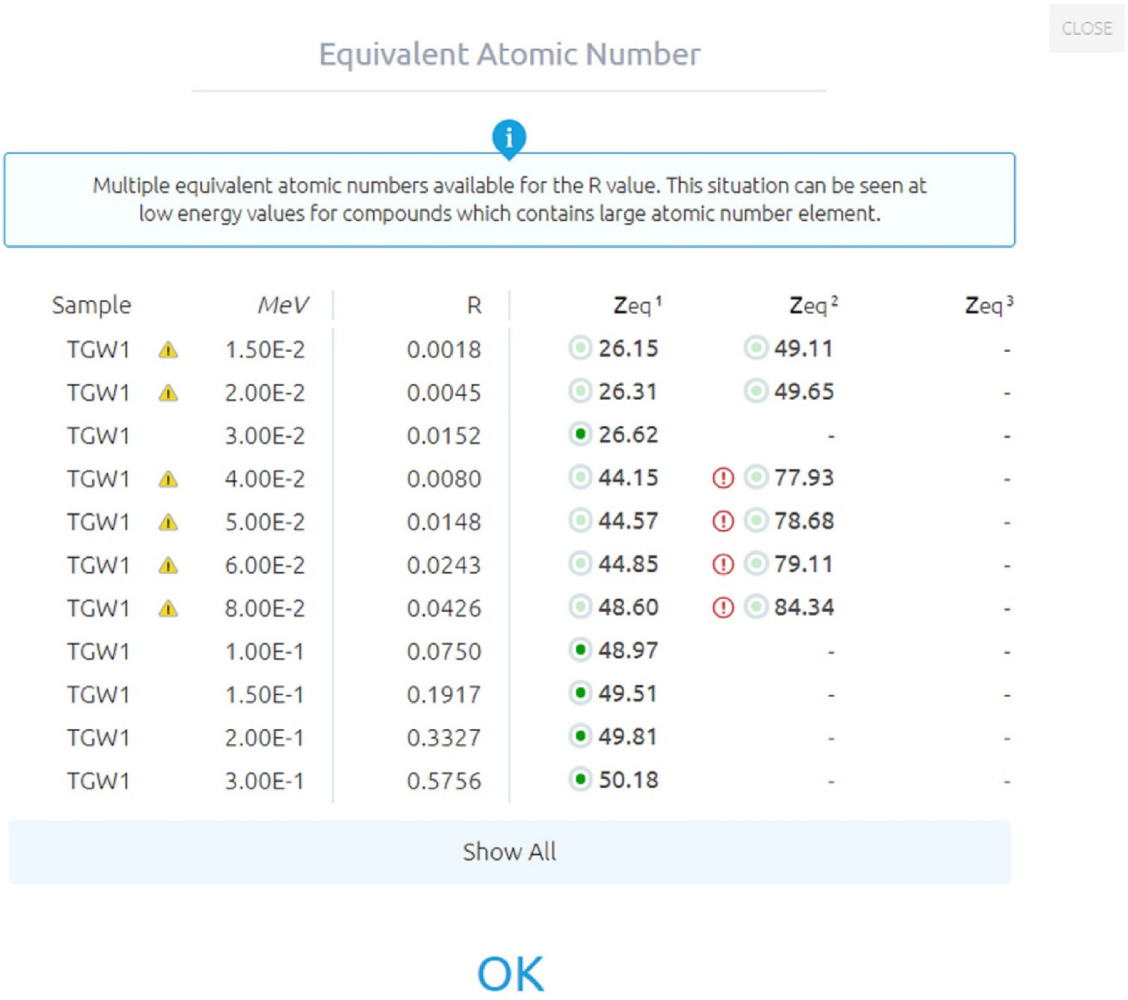

Fig. 7. The selectable Z_{eq} values in the PSD online software.

4. Results and discussion

There is a tremendous interest on studies of X- and gamma ray interaction with different media. These data are strictly required in many engineering and medical applications particularly in radiation protection and dosimetry fields. The quantities such as MAC, HVL, MFP, Z_{eff}, and C_{eff} which demonstrate the radiation shielding performance of the materials and help in the selection of the best shielding material in related technological fields, are called radiation shielding parameters, and the correct calculation of these parameters is mandatory for the characterization of the shielding materials in shielding and dosimetry calculations. Furthermore, when designing any shielding material, the radiation shielding parameters of this material must be calculated both experimentally and theoretically and these results obtained must be compatible with each other. Given that these parameters are calculated in a wide energy range; a huge amount of data need to be compiled. In this regard, manual calculations are really time-consuming and sometimes handmade calculations lead to calculation errors. According to the literature review, researchers prefer computer-based theoretical software such as WinXCOM (Gerward et al., 2004) and GEANT4 (Agostinelli et al., 2003) in order to make calculations free of errors, reduce the time needed for calculations and minimize the use of consumable in the experimental phase. However, these useful computer software can only calculate the MAC values of the materials, they cannot calculate all the shielding parameters given in Table 3. Therefore, it is clear that a theoretical-based software that can calculate all radiation shielding parameters in a fast, practical, accurate and comparative manner is required in the selected or continuous wide energy range.

In this study, a user friendly PSD online software has been developed which can meet the all requirements mentioned above and calculate all radiation shielding parameters in the wide energy range which is given in section 3.2 for any materials. In addition to these calculations, the software can generate another parameter relevant to shielding i.e. the fast neutron removal cross section (FNRCS). The shielding of fast neutrons is very important for nuclear applications. A reliable solution to the evaluation of the neutron-shielding capacity of any materials is based on determination of accurate values for fast neutron removal cross sections. For this reason, calculation of FNRCS values have been added to the developed software. Some example calculations of FNRCS can be found in supplementary file.

The output data obtained through the proposed software (processing time is about 17 s) has been compared with the available data in literature. A comparison for MAC data with those of Önder et al. (Onder et al., 2012) has been made for $MgSO_4$ and the results have been shown in Fig. 5a. It is seen that data produced through the software agree well with those already published.

For the purposes of photon attenuation, a composite material, consisting of a number of elements in varying proportions, can be specified as imaginary element having an effective atomic number (Z_{eff}). Similarly, in scattering interactions, the parameter that characterizes the entire material depending on the energy of the incoming photon is Z_{eq}. While Z_{eff} is all about the total attenuation including scattering and absorption processes, Z_{eq} is about the scattering process only. In addition, while the Z_{eff} parameter has the highest values in the photoelectric region where absorption is dominant, Z_{eq} takes maximum values in the region where Compton scattering is dominant. A comparison has been made for G-P fitting parameters as well as for Z_{eq} (Fig. 6a–f) and Z_{eff} (Fig. 5b). The software produced values (processing time is about 42 s) have been compared with those available for $70BaO{:}30SiO_2$ material (Singh et al., 2014). The results indicate that our results compare very well with those of Singh et al. (2014). The comparison of G-P fitting, Z_{eq} and Z_{eff} values for both Singh's results and Phy-X/PSD results are given in Table 4. Furthermore, absolute deviations of the aforementioned results can be seen in Table 5.

For the evaluation of buildup factors, the equivalent atomic number (Z_{eq}) needs to be calculated first. It is obtained using a logarithmic interpolation based on interpolating the R values with the R values of adjacent elements (see Eq. (12) and (13)). It has to be noted that the Z_{eq} must take values between the lowest and highest atomic number constituting the material. Somehow, more than one range satisfying the above condition can be obtained. In this case, software determines the ranges and different values of Z_{eq} satisfying the above condition and leave it to the user to decide which range, thus Z_{eq} should be used in calculations. An example calculation of Z_{eq} was done for the composition of 82.5TeO2 + 10GeO2 + 7.5WO3 (Fig. 7). It is clearly seen that the obtained R value corresponds to two different Z_1 and Z_2 range. Since there is no selection rules for this parameter in the literature, the selection of this value is left to the user's choice.

5. Conclusion

In this study, a user friendly PSD online software available at https://phy-x.net/PSD has been developed for calculation of all parameters relevant to shielding and dosimetry. It works on a NodeJS platform and give the results in a reasonably quick time period depending on the number of calculations. For example, as it can be seen in the supplementary files, the software makes around 377600 calculation counts in about 500 seconds for four different materials. The software can generate data on LAC, MAC, HVL, TVL, MFP, ACS, ECS, Z_{eff}, N_{eff} and C_{eff} in the wide energy range of 1 keV–100 GeV. Additionally, a set of well-known radioactive sources (^{22}Na, ^{55}Fe, ^{60}Co, ^{109}Cd, ^{131}I, ^{133}Ba, ^{137}Cs, ^{152}Eu and ^{241}Am) and some characteristic X-ray energies (the K-shell energies of Cu, Rb, Mo, Ag, Ba and Tb elements) have been predefined in the software. Moreover, the EABF and EBF values and fast neutron removal cross-sections (FNRCS) for any selected material can be calculated by the software. The most important feature of this developed software is that it can simultaneously calculate all the shielding and dosimetric parameters mentioned above in a fast and accurate way for an infinite number of different materials. Another important feature is that the user is free to choose the desired parameters from all given shielding parameters and can save data in a MS Excel file that is designed in a very understandable and practical form. The accuracy of the developed PSD program has been checked by comparing values with those available in literature. The software is freely available for users satisfying the citation conditions when using this software. It is expected that this program will help researchers to develop low cost and reliable shielding materials by making accurate calculations in all shielding studies in a short time period.

Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.radphyschem.2019.108496.

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