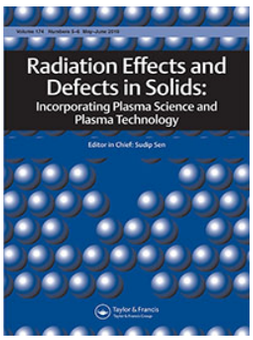

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Radiation Effects and Defects in Solids
Incorporating Plasma Science and Plasma Technology

ISSN: 1042-0150 (Print) 1029-4953 (Online) Journal homepage: https://www.tandfonline.com/loi/grad20

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To cite this article: Önder Eyecioğlu, A. M. El-Khayatt, Yaşar Karabul, Mustafa Çağlar, Ozan Toker & Orhan İçelli (2019) BXCOM: a software for computation of radiation sensing, Radiation Effects and Defects in Solids, 174:5-6, 506-518, DOI: 10.1080/10420150.2019.1606811

To link to this article: https://doi.org/10.1080/10420150.2019.1606811

Published online: 24 Apr 2019.

RADIATION EFFECTS & DEFECTS IN SOLIDS
2019, VOL. 174, NOS. 5–6, 506–518
https://doi.org/10.1080/10420150.2019.1606811

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BXCOM: a software for computation of radiation sensing

Önder Eyecioğlu[a], A. M. El-Khayatt[b,c], Yaşar Karabul[d], Mustafa Çağlar[e], Ozan Toker[d] and Orhan İçelli[d]

[a]Department of Computer Engineering, Engineering and Architecture Faculty, Nisantasi University, Istanbul, Turkey; [b]Physics Department, College of Science, Imam Mohammad Ibn Saud Islamic University (IMSIU), Riyadh, Saudi Arabia; [c]Reactor Physics Department, Nuclear Research Centre, Atomic Energy Authority, Cairo, Egypt; [d]Department of Physics, Science and Art Faculty, Yıldız Technical University, İstanbul, Turkey; [e]Institute of Health Sciences, Department of Medical Physics, Istanbul Medipol University, İstanbul, Turkey

ABSTRACT

The main objective of this work is to develop user-friendly software, called BXCOM, for computation of the exposure build-up factor (EBF) and the energy absorption build-up factor (EABF), using geometric progression (G-P) fitting method for element, compound or mixture in the energy region 0.015–15 MeV, and for penetration depths up to 40 mean free path (mfp). Furthermore, BXCOM can generate the equivalent atomic number (Z_{eq}) and five fitting parameters used in the G-P method for mixtures and compounds over an interval of photon energies extended from 0.015 to 15 MeV. In addition, the program is designed to calculate the effective atomic number (Z_{eff}) and effective electron number (N_{eff}) via the direct method. BXCOM program has been verified by comparing its results with approved data by American National Standards Institute. BXCOM runs under MS Windows® operating system. It has an improved user interface that provides examination of material's radiation interaction parameters. Finally, BXCOM allows rapid and reliable calculation of many γ-ray interaction parameters such as (Z_{eq}), (Z_{eff}), (N_{eff}), G-P fitting parameters and build-up factors that are essential in a wide range of applications such as radiation shielding, radiotherapy, technology and so on.

ARTICLE HISTORY
Received 22 January 2019
Accepted 23 March 2019

KEYWORDS
Energy absorption build-up factor; exposure build-up factor; BXCOM; software

1. Introduction

Build-up factor has a significant role in dispersion of photons (*1*). It determines the degree of violation of the Lambert–Beer law with the uncollided flux and predicts the total flux. It is a correction factor considers secondary particles and distribution of collided photons. Thus the ratio of the total detector response to the uncollided photons can be determined (*2*). The Build-up factor can be categorized into two fundamental groups: exposure build-up factor (EBF) and energy absorption build-up factor (EABF). For EBF, it is assumed that the detector response function is equivalent to the amount absorbed in the air measured by the non-perturbation detector. EABF is the build-up factor in which the quantity of interest is the deposited energy in the absorber material or medium (*3*). Information on EBF and

CONTACT Orhan İçelli oicelli@yildiz.edu.tr

EABF is important in radiation therapy and dosimetry to analyze the energy deposition in a medium exposed to γ or X-rays (*4*). Generally, the build-up factor is included as a correction factor to take into account the γ-ray attenuation problem.

Approved EBF–EABF values for water, air and concrete were represented by The American National Standards Institute (*5*). The ANSI/ANS-6.4.3 lists build-up factor values for 23 elements ($Z = 4$–92), water, air and concrete. In addition, Harima developed the geometric progression (G-P) fitting formula as defined in Equations (10)–(12) (*6*). Fitting variables in the G-P process show suitable results with the ANSI/ANS. The G-P fitting method can accurately reproduce the build-up factors over the full range of distance, energy and atomic number with a few percent error (*6*, *7*). Later, it was adopted by ANS-6.4.3-1991 as the best available form for the fitting function. In fact, the standard was administratively withdrawn because of the inconsistency. It is suggested that the use of the 1991 standard should be appropriate for low-and medium-Z materials (*8*) and it should be updated for materials with a high atomic number (*9*).

The subject of build-up factors has been studied extensively both experimentally and theoretically by many authors over the last few decades. For example, Uei et al. studied experimentally the build-up factor for a point isotropic source in stratified spherical shields (*10*). Also, Aljundi and Gray proposed a new set build-up factors for the X-ray radiography which approximate the effect of scattering in the white spectrum of incident radiation (*11*). In addition, they measured experimentally these proposed factors and modulated a Monte Carlo code to reproduce the experimentally measured values.

To calculate the value of build-up factor, there are a variety of computational methods like G-P fitting method (*12*), the method of adjoint γ-moments (*13*), iterative method (*14*) and the direct integration of transport equation method (*15*), Monte Carlo method (*16*) and artificial neural networks (*17*). In addition, Hirayama calculated the γ-ray EBFs up to 40 mfp using the Monte Carlo code EGS4 with a new algorithm which implements particle splitting at a selected depth in order to obtain reasonable results with EGS4 at deep penetration (*18*).

Shimizu et al. reported a comparison among the build-up data which determined with three common methods: Monte Carlo, invariant embedding and G-P fitting methods for low-Z elements for different mean free paths (up to 100 mfp) (*19*). In addition, Fujisawa examines the calculation accuracy of different codes, which based on various methods such as QAD and MARMER (a point-kernel method), ANISN (a discrete ordinate method) and MCNP method (*20*). The G-P fitting formula is admissible to be accurate within the estimated error ($< 5\%$) (*7*).

In spite of the rapid growth of the computational work of build-up factors, there is no software available for calculating the EABF and EBF by G-P fitting formula. This prompted us to carry out this study. The main aim of this study is to develop an effective and valid tool to calculate the EABF and EBF factors using the G-P fitting method. This tool called BXCOM program which calculates these parameters for any element, compound or mixture under various conditions (incident photon energy; $0.015 \leq E_0 \leq 15$ MeV and depths up to 40 mfp). The interpolation method was utilized to estimate the EABF and EBF values. This process can be used for the analysis of the interrelated data since it never affects the elemental distribution.

It is reported that the parabolic interpolation method can be used to determine G-P fitting parameters with (Z_{eff}) by Harima (*12*), however, using of (Z_{eq}) is the most common method for materials. In addition, Harima noticed that the different energy ranges

effect (Z_{eq}) values for materials (above or below 1.5 MeV) (*12*). This has prompted some researchers to determine fitting parameters using the interpolation of effective atomic number (*21*) rather than the equivalent atomic number. So, our software lists both values of (Z_{eff}) and (Z_{eq}) for preferred compound or mixture.

The BXCOM program has a dynamical graphical user interface (GUI) and runs under MS Windows operating systems. With this GUI, the outputs can be tracked in real time as well as it provides an examination of a material's radiation interaction parameters as follows:

1. The mfp parameter is considered as dynamic variable; dynamic variables are useful for viewing data under various experimental conditions.
2. (Z_{eff}), (N_{eff}), (Z_{eq}), EABF and EBF of the studied material are generated on the predefined energy grid.
3. The output results can be generated in an MS Excel file and shown in a variety of dynamic graphics formats such as JPG, PNG and so on.
4. The program output also presents the G-P fitting parameters as a text file.

2. Theoretical method

2.1. Effective atomic number (direct method)

An effective atomic number can be determined via two different methods: a direct method (*22*) and an interpolation method (*23*). Manohara et al. reported a comparative study of these numerical methods (*24*). They stated that the direct method has more accurate results than the interpolation method. Stages of determination of (Z_{eff}) by the direct method are based on the assumption that σm (molecular cross-section) can be expressed depending on σa (average atomic cross-section) and σe (an average electronic cross-section), like

$$\sigma_m = n\sigma_a = nZ_{eff}\sigma_m. \tag{1}$$

The details of the calculations are given in other sections.

2.1.1. The total molecular cross-section

In order to determine total molecular cross sections ($\sigma_{t,m}$), mass attenuation coefficients can be used as in Equation (2).

$$\sigma_{t,m} = \frac{1}{N}\left(\frac{\mu}{\rho}\right)_{comp}\sum_i (n_i A_i). \tag{2}$$

Here, the total mass attenuation coefficient is represented with $\left(\frac{\mu}{\rho}\right)_{comp}$. Besides, atomic weight, Avogadro's number and a number of the atoms of the *i*th element in a molecule are represented with A_i, N and n_i, respectively.

2.1.2. The total atomic cross-section

$\sigma_{t,a}$ (total atomic cross-section) can be defined as

$$\sigma_{t,a} = \sigma_{t,m}\frac{1}{\sum_i n_i}. \tag{3}$$

2.1.3. The total electronic cross-section

$\sigma_{t,e}$ (total electronic cross-section) for the certain element is expressed by Equation (4):

$$\sigma_{t,e} = \frac{1}{N}\sum_i \frac{f_i A_i}{Z_i}\left(\frac{\mu}{\rho}\right)_i. \tag{4}$$

Here Z_i is the atomic number of the ith element in a molecule and $\left(\frac{\mu}{\rho}\right)_i$ is the total mass attenuation coefficient of the ith element in a molecule, also, f_i is the number of atoms of element ith relative to the total number of atoms of all elements in the mixture.

2.1.4. The effective atomic number

The definition of (Z_{eff}) is given in Equation (1)

$$Z_{eff} = \frac{\sigma_{t,a}}{\sigma_{t,e}}. \tag{5}$$

2.1.5. Electron densities (electrons/g)

The definition of (N_{eff}) is given in Equation (6)

$$N_{eff} = \frac{Z_{eff}}{A_{top}}(N\, n_{top}), \tag{6}$$

where A_{top} is the total number of the atomic weight for material.

3. Build-up factor origin

The Lambert–Beer Law ($I = I_0 e^{-\mu x}$) can only be applied if three conditions are met: (i) the radiation source must be monoenergetic, (ii) for a single interaction between photon and material, the target (iii) irradiation beam must be narrow. If one of these conditions is not met, the Lambert–Beer Law must be modified. The modified Lambert–Beer Law is

$$I = BI_0 e^{-\mu x}. \tag{7}$$

The build-up factor is represented by B. The transmitted $(I_{measured})$ and incident (I_0) intensities of photons for various elements, compounds and mixtures were recorded. The calculations of the transmitted intensity $(I_{calculated})$ for incident intensity (I_0) were performed with the Lambert–Beer Law. It was noticed that the value of $I_{measured}$ is always greater than $I_{calculated}$ and the build-up factor (*3*).

3.1. Exposure and energy absorption build-up factors

Using of a (Z_{eq}) is the common adopted method of the G-P fitting factor coefficients (or fitting parameters) in Z for materials. (Z_{eq}) is a parameter that varies depending on the incident energy. It was employed to describe the properties of materials in terms of equivalent elements. Harima reported a calculation method for estimating (Z_{eq}) for mixtures and compounds.

Compton cross-section to the total cross-section ratio (μsc/μtot) provides to determine (Z_{eq}) values of the materials for a certain energy (*6*). First, determination of the μsc/μtot

ratios was performed for 23 different elements (atomic numbers are 4–92) and for the different energy values from 0.015 to 15 MeV. These calculations were carried out via WinXCom software (*25*). Parabolic interpolation can be performed for determination of the (Z_{eq}) values by using Equation (8). After, interpolation can be performed for the determination of G-P fitting parameters, and the final stage of the calculations is the determination of the build-up factors. All the calculations were summarized as below:

i. Determination of Z_{eq} (equivalent atomic number)
ii. Determination of G-P fitting parameters (geometric progression) and
iii. Determination of EBF (exposure build-up factors) and EABF (energy absorption build-up factors).

A calculation method for equivalent atomic number Z_{eq} has been described elsewhere (*26*–*28*). In general, the following equation can be used to interpolate

$$Z_{eq} = \frac{Z_1(\log R_2 - \log R) + Z_2(\log R - \log R_1)}{\log R_2 - \log R_1}. \tag{8}$$

Here, Z_1 and Z_2 are the atomic numbers of the elements used for interpolation, R_1 and R_2 are the values of the μ_{sc}/μ_{tot} ratios for the same elements and R is the corresponding ratio for the studied material.

This calculation method can be confirmed with an example: the R (corresponding ratio) for H_2O that interacts with photons with 0.015 MeV energy can be determined as $R = 0.1104$ (μ_{sc}/μ_{tot} for H_2O), which should be compared with $R_1 = 0.1329$ and $R_2 = 0.0862$ for the elements $Z_1 = 7$ and $Z_2 = 8$. It follows from Equation (8) that $Z_{eq} = 7.43$.

After, in order to determine the G-P fitting parameters, similar interpolation process can be performed by using the equivalent atomic number. ANSI/ANS-6.4.3 standard reference database represents the G-P fitting parameters for elements from Be to Fe (0.015–15 MeV energy range and up to 40 mfp). Thus Equation (9) can be performed for the interpolation of the G-P fitting parameters

$$C = \frac{C_1(\log Z_2 - \log Z_{eq}) + C_2(\log Z_{eq} - \log Z_1)}{\log Z_2 - \log Z_1}. \tag{9}$$

Here, C_1 and C_2 correspond to the coefficients related to Z_1 and Z_2 to the atomic numbers of respectively. In addition to Z_{eq} is the equivalent atomic number of the material studied. At the final step, these parameters can be used to calculate the exposure and energy absorption build-up factors from the G-P fitting formula:

$$B(E,X) = \frac{b-1}{K-1}(K^x - 1) \text{ for } K \neq 1, \tag{10}$$

$$B(E,X) = 1 + (b-1)x \text{ for } K = 1. \tag{11}$$

Here, x represents the penetration depth in the medium in unit of mfp. (b) represents the value of the build-up factor at 1 mfp (*5*). Photon dose multiplication is represented by K.

This parameter can be defined as a function of E and x as follows:

$$K(E,x) = cx^a + d\frac{\left[\tanh((x/X_k) - 2) - \tanh(-2)\right]}{\left[1 - \tanh(-2)\right]}. \quad (12)$$

Here incident photon energy is represented by E. Fitting parameters are given by a, b, c, d and X_k.

3.2. Mean free path

A mean free path is a unit of the penetration depth of radiation interacting material. The mfp represents the mean distance between two interactions of photons. This distance causes a decrease in the intensity of the incident photon beam by the factor of $1/\mu$ (μ : linear attenuation coefficient). Energy of the incident photon affects the mean free path and the linear attenuation coefficient.

4. The BXCOM software

The BXCOM program determines (Z_{eff}), (Z_{eq}), EABF, EBF and G-P fitting parameters for any element, compound or mixture, at incident photon energies from 15 keV to 15 MeV. The BXCOM runs under MS Windows-based operating systems. Object-Oriented Programming (OOP) language called Visual C# has been used for codding. BXCOM includes 10 classes: photon, elements, compound, mixture, periodic table, formula, formula components, mathematics, form and main classes. The object model and class organization of the program is given in Figure 1 as an UML diagram.

The photon class is to control the incident photon energy (in MeV) and depth (in mfp). The most important class structure of the program is element class. All required elemental data such as atomic number, atomic mass and interaction coefficients are stored in element class. Also, the element class computes various elemental parameters such as(Z_{eff}), (Z_{eq}), G-P fitting parameters, EABF and EBF factors. The compound and mixture classes are estimated from element class by the aid of formula objects, which is generated by formula and formula component classes. All necessary mathematical equations are stored in the mathematic class where the interpolation process is done.

The GUI is created by Form class and is shown in Figures 2–4. All calculations are made for the studied samples in the energy range 0.015–15 MeV and up to 40 mfp. A preferred element in the periodic table can be selected easily by clicking on the element tab that located in the left side of the GUI (Figure 2). Similarly, any compound (Figure 3) or mixture (Figure 4) can be easily defined through writing the chemical formula of the compound.

The main outputs of the BXCOM program are (Z_{eff}), (Z_{eq}), EABF, EBF and G-P fitting parameters which vary according to incident photon energy and penetration depth. (Z_{eff}), (Z_{eq}), EABF and EBF are listed with a 'datagridview' object that located right side of the GUI as seen in Figures 2–4. The table of the data that listed in the 'datagridview' object can be exported to the MS Excel template. The G-P fitting parameters can be stored in a text file via the Open File Dialog method. In addition, the graphs of the obtained data are dynamically graphed, during the ongoing run, onto the top side of the GUI. The graphs can be saved in one of the many image formats such as JPEG, PNG, TIFF and so on.

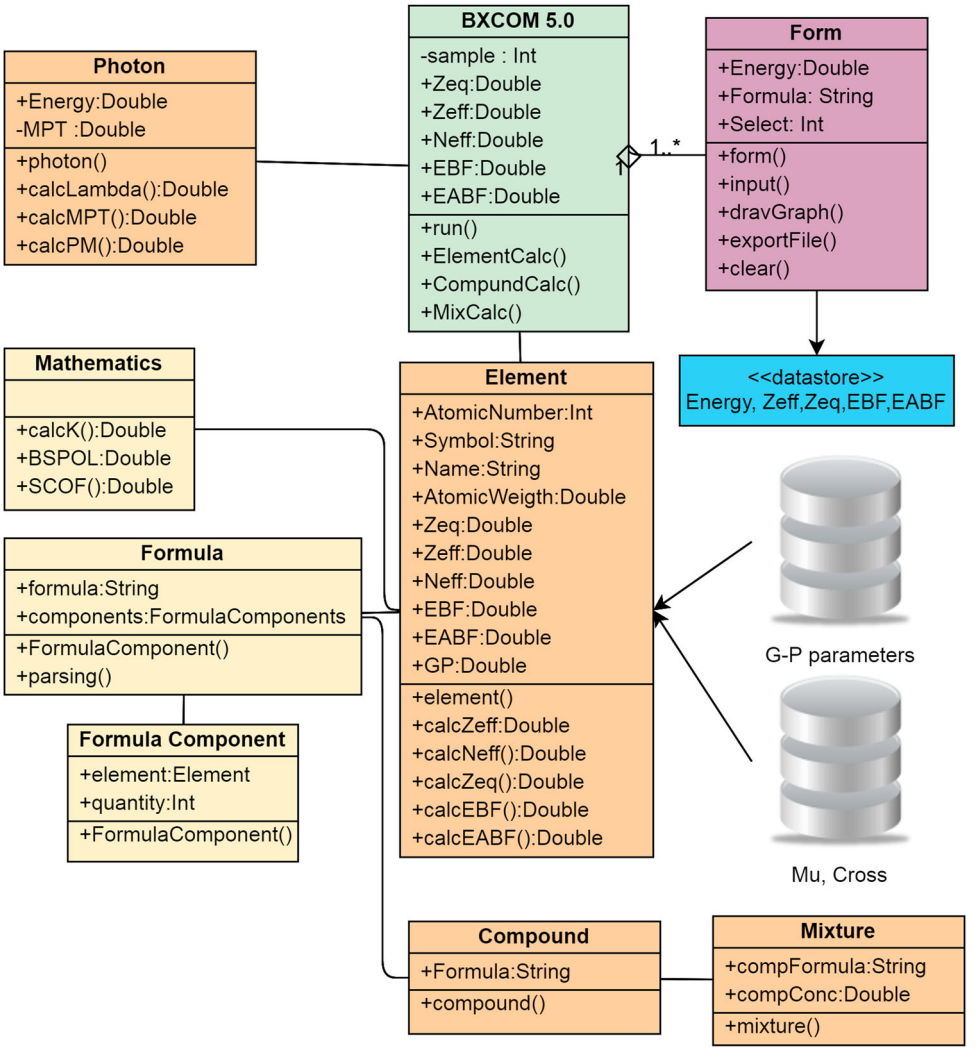

Figure 1. Unified modeling language (UML) class diagram of BXCOM.

MS Windows operating system (32-bit or 64-bit) 232 is a suitable platform for the BXCOM program. BXCOM Install file provides the installation of the program as seen in Figure 5. Interested readers can easily and freely download the setup file from http://photon.yildiz.edu.tr/BXCOM.php.

In summary, (Z_{eff}) and (Z_{eq}) of the selected materials are determined by the direct method as defined by Manohara (*22*) and by the interpolation method as described by Harima (*6*), respectively.

The total mass attenuation coefficients (μ/ρ) used for the calculation of (Z_{eq}) in the energy range 0.015–15 MeV are obtained by using the WinXCom computer program (*25*). Then, the interpolation procedure, as described in Equation (9), was adopted to calculate the G-P fitting parameter, corresponding to the computed (Z_{eq}). Finally, the exposure and energy absorption build-up factors are calculated using Equations (10)–(12).

Figure 2. A view of BXCOM GUI while it computes elements.

Figure 3. A view of BXCOM GUI while it computes compounds.

5. Program verification

In order to verify the reliability of the software, *i.e.* that software is capable of performing a failure-free operation, we have compared the obtained results for EABF values for water with those calculated via the G-P method, which can be found elsewhere (*29*). Figure 6 shows the compared values of EABF for certain energies and different penetration depth. It can be seen from Figure 6 that the EABF values generated by the software are in good agreement with the G-P results. This gives confidence in the generated results.

On the other hand, in order to standardize the G-P fitting formula, which employed in the BXCOM program, we have computed energy absorption build-up factors of water

Figure 4. A view of BXCOM GUI while it computes mixture.

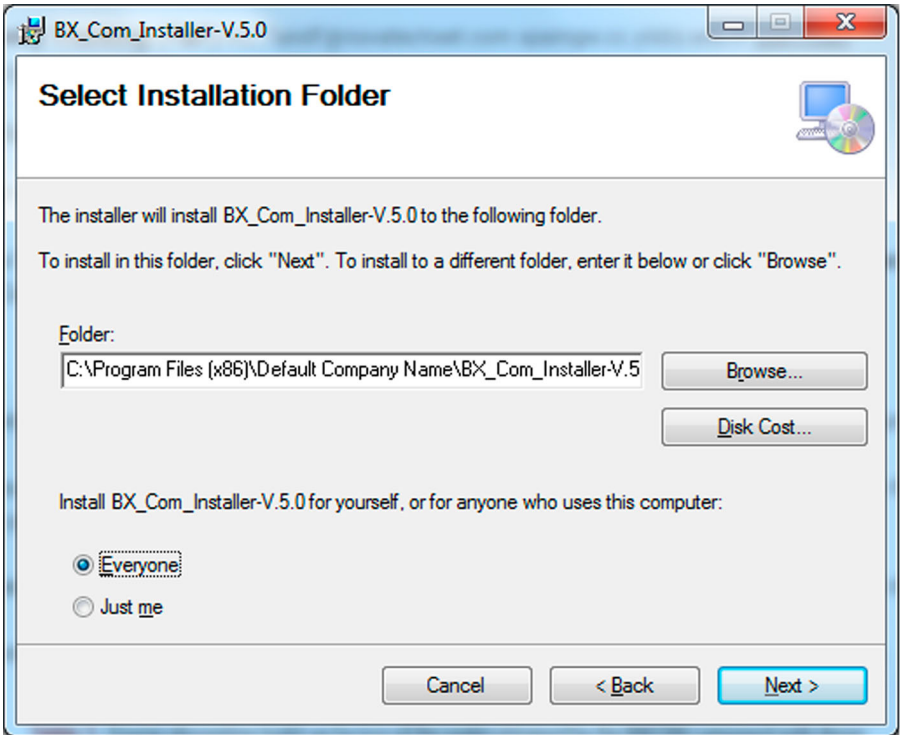

Figure 5. Install setup wizard of the BXCOM program.

by the program for the certain energies (0.015–15 MeV) and different penetration depth. Thus comparison of determined values was performed with ANSI/ANS-6.4.3 data and values were updated for low-Z and compound materials which reported by Durani (*30*).

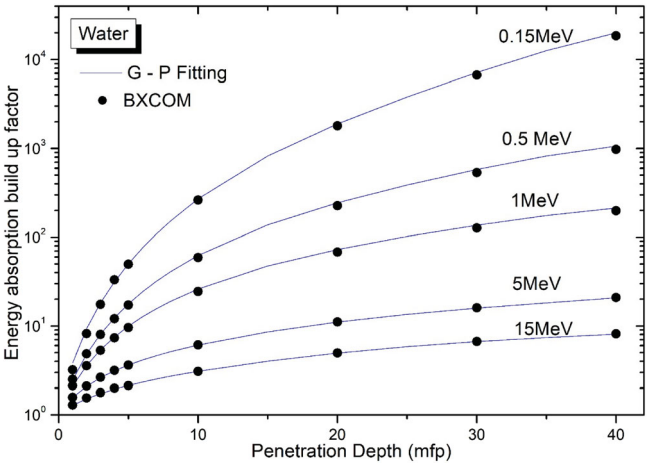

Figure 6. Energy absorption build-up factors of water computed by BXCOM (circles) compared with those calculated by the G-P fitting method (solid line) taken from Manohara et al. (*29*).

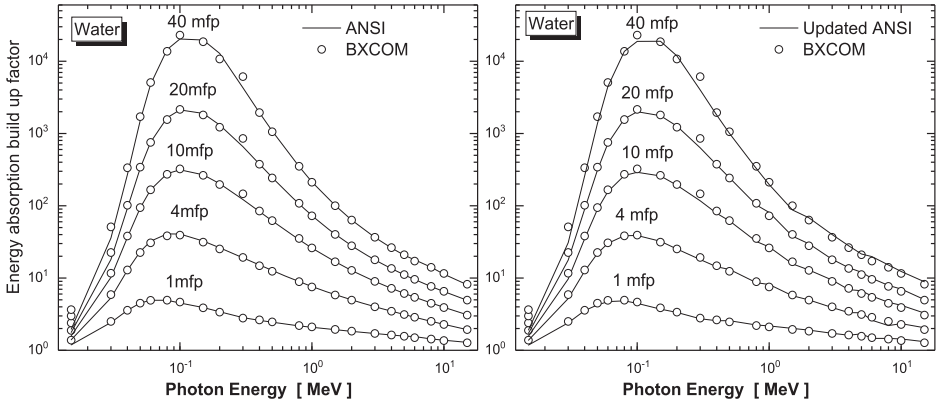

Figure 7. Energy absorption build-up factors of water calculated by BXCOM (circles) compared with those of the ANSI standard and its update (solid line) at certain penetration depths (in mfp); updated ANSI values were taken from Durani (*30*).

Figure 7 shows the photon energy dependence of the EABF values determined by the program for water. It also shows the EABF values approved by American National Standards Institute and its update values (*30*) for different penetration depths (up to 40 mfp). It is observed that the results determined by BXCOM program are compatible with the standard data and its updated values.

Table 1 lists the BXCOM results of EABF for water with those of ANSI standard and the results of applying of G-P method at photon energies 0.5–15 MeV. The percentage deviation is less than 3%. This means that the EABF generated by BXCOM, which based on G-P fitting formula, are in good agreement with those given by ANSI standard.

Figure 8 shows the photon penetration depth dependence of the EABF for water, as computed by the BXCOM and the values approved by American National Standards Institute at

Table 1. Energy absorption build-up factors of the water obtained by the BXCOM compared with those of the ANSI/ANS-6.4.3 standard and G-P fitting formula.

				% deviation					% deviation	
x (mfp)	ANSI	G-P[a]	BXCOM	ANSI	G-P	ANSI	G-P[a]	BXCOM	ANSI	G-P
	Energy = 0.5 MeV					*Energy = 1 MeV*				
1	2.45	2.47	2.47	−0.95	−0.13	2.08	2.11	2.10	−1.18	0.26
2	4.87	4.84	4.84	0.71	0.09	3.62	3.59	3.59	0.84	0.01
3	8.29	8.12	8.11	2.18	0.13	5.5	5.41	5.40	1.78	0.14
4	12.7	12.4	12.37	2.57	0.21	7.66	7.54	7.53	1.75	0.19
5	18.1	17.76	17.71	2.17	0.30	10.1	9.97	9.95	1.51	0.22
10	61.8	62.57	62.21	−0.66	0.58	26	26.16	26.06	−0.21	0.40
20	247	244.31	242.33	1.89	0.81	73.5	72.87	72.46	1.42	0.57
30	582	579.99	574.38	1.31	0.97	138	136.84	136.13	1.35	0.52
40	1080	1067.38	1057.31	2.10	0.94	214	213.56	211.13	1.34	1.14
	Energy = 5 MeV					*Energy = 15 MeV*				
1	1.57	1.57	1.56	0.40	0.40	1.29	1.28	1.27	1.38	0.61
2	2.10	2.10	2.10	0.10	0.10	1.51	1.52	1.51	0.11	0.76
3	2.62	2.62	2.62	0.14	0.14	1.72	1.74	1.73	−0.37	0.79
4	3.12	3.13	3.12	−0.15	0.17	1.93	1.94	1.93	−0.13	0.39
5	3.63	3.64	3.63	0.09	0.36	2.14	2.14	2.13	0.43	0.43
10	6.14	6.10	6.10	0.58	−0.07	3.11	3.08	3.07	1.28	0.31
20	11.10	11.06	11.14	−0.39	−0.76	4.93	4.94	4.95	−0.44	−0.24
30	15.90	15.91	16.04	−0.89	−0.83	6.64	6.66	6.69	−0.81	−0.51
40	20.70	20.73	21.02	−1.56	−1.41	8.09	8.11	8.19	−1.26	−1.01

[a]The values were taken from by Manohara et al. (*29*).

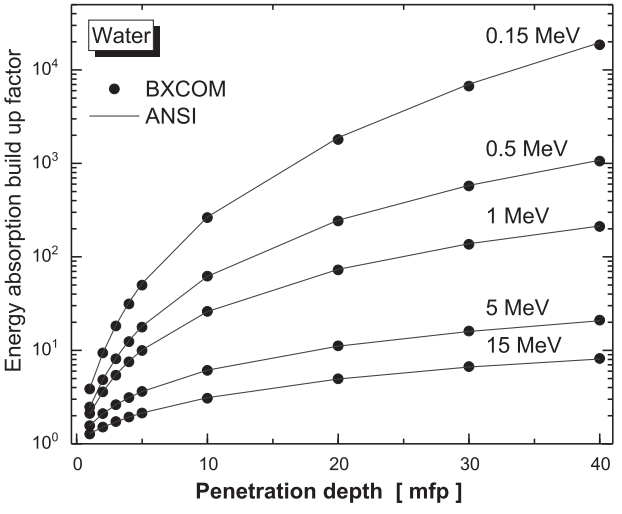

Figure 8. Energy absorption build-up factors of water computed by BXCOM (circles) compared with ANSI standard data (solid line), at some selected energies in MeV.

different certain photon energies. From Figures 7 and 8, it is obvious that the EABF values determined with software are compatible with the literature with respect to the photon energy and the photon penetration depth. This means that the BXCOM program results can be trusted in calculations for different materials.

6. Conclusion

The authors designed and verified a computer program, called BXCOM, which utilizes the well-known G-P fitting formula to obtain (Z_{eff}) and (Z_{eq}), EABF, EBF and G-P fitting parameters. It also calculates the effective atomic number of any compound or substance in the energy region extended from 0.015 to 15 MeV. When the user enters the material of interest, and the desired penetration depth, the software will generate tables and graphs for EABF and EBF; arranged in ascending order based on the photon energy and provides the G-P fitting parameters as a text file. BXCOM facilitates computation of the EABF, and the EBF as a function of photon energy, as well as a function of photon penetration depth. The using of the BXCOM program prevents the user from making time-consuming and error-free calculations and provides to store, manage and analyze the determined data through an Excel template file. This software is both flexible and rapid, requiring approximately less than 7 s of computing time. The program is expected to be helpful to develop new shielding materials, radiation dosimetry, diagnostics and radiotherapy.

Disclosure statement

No potential conflict of interest was reported by the authors.

Funding

This work was supported by Türkiye Bilimsel ve Teknolojik Araştırma Kurumu [Grant Number 2015-115F311].

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