Semi-empirical formula for photon energy absorption buildup factors of elements and compounds

H.C. Manjunatha*

Department of Physics,
Government College for Women,
Kolar-563101 Karnataka, India
Email: manjunathhc@rediffmail.com
*Corresponding author

L. Seenappa

Department of Physics,
Government College for Women,
Kolar-563101 Karnataka, India
Email: seenappakolar@gmail.com

K.N. Sridhar

Department of Physics,
Government First Grade College,
Kolar-563101 Karnataka, India
Email: knsphy@gmail.com

Abstract: We have formulated a simple semi-empirical formulae for photon energy absorption buildup factors in the energy region 0.015–15 MeV, atomic number range $1 \leq Z \leq 92$ and for mean free path up to 40 mfp. The results produced by the present formulae agree well with the data available in the literature. This semi-empirical formula may be extended to any compounds/mixtures/biological samples. This semi-empirical formula finds importance in the calculations of buildup factors of any materials which are required for radiation shielding, nuclear engineering, radiotherapy and nuclear medicine.

Keywords: fast reactors; sodium-cooled reactor; breed and burn; metallic fuel; ASTRID.

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Biographical notes: H.C. Manjunatha is an Assistant Professor of Physics at Government College for Women, Kolar, Karnataka, India. His areas of research are radiation, nuclear and medical physics. He has published more than 100 research papers in reputable international journals. He has also served as reviewer for many international journals.

L. Seenappa is an Assistant Professor of Physics at Government College for Women, Kolar, Karnataka, India. His areas of research are radiation and medical physics. He has also published more than 25 research papers.

K.N. Sridhar is an Assistant Professor at Government First Grade College, Kolar. His areas of research are nuclear and radiation physics. He has also published more than 30 research papers.

1 Introduction

The buildup factors are used in shielding calculations, nuclear medicine and nuclear engineering. The buildup factor is defined as the ratio of total intensity to the intensity of un-collided photons. There are two types of buildup factors viz exposure buildup factor and energy absorption buildup factor. Energy absorption buildup factor is that in which it represents the absorbed or deposited energy in the material/medium. Exposure buildup factor is that in which it represents the energy deposited in the air (exposure).

These buildup factors determined are useful in radiation dosimetry, medical diagnostics and therapy, space dosimetry, accident dosimetry and personnel monitoring. Previous workers studied the absorption buildup factors in the materials which are used in the radiation protection and radiation biology (Hernández and El-Daoushy, 2002; Singh and Badiger, 2014; Kavaz et al., 2015; Mann et al., 2016; Levet and Özdemir, 2017; Singh and Badiger, 2014). Detailed literature survey shows that there is some investigation of absorption buildup factors in compounds which are used as drugs (Ekinci et al., 2014; Kurudirek and Topcuoglu, 2011). Park and Jeong (2016) analysed uncertainties in the weighted least squares fitted buildup factors in the point kernel method. Most of the researchers studied the energy absorption buildup factors using the geometric progression method (Kurudirek and Özdemi, 2011; Manohara et al., 2010; Mann et al., 2012; Kurudirek et al., 2011; Singh et al., 2018; Mann and Korkut, 2013; Sharaf and Saleh et al., 2015; Sardari et al., 2009; Singh et al., 2015; Manjunatha and Rudraswamy, 2012a, 2012b, 2011a; Singh et al., 2014; Kucuk, 2008; Singh et al., 2010; Kaur et al., 2012; Brar et al., 1994; Brar and Mudahar, 1996; Brar et al., 1998; Manjunatha and Rudraswamy, 2011b). It is also evident from the literature that there are a few researchers who studied energy absorption buildup factors using some other methods such as neural network and MCNP codes (Kucuk et al., 2013; Atak et al., 2015; Kucuk, 2010; Aten Jr., 1978; ANSI/ANS-6.4.3, 1991).

Experiments aimed at obtaining buildup factors are generally not easy. From the literature survey, it is clear that most of the researchers employed GP fitting method (ANSI/ANS-6.4.3, 1991) to compute the energy absorption buildup factors. This method requires a number of coefficients which depends on photon energy, mean free path and atomic number. Hence, this GP fitting method requires a bulky data. There is a need to develop a simple method/relation to calculate a photon buildup factors. The aim of this paper is to establish a simple relation for photon energy absorption buildup factors. In this paper, we have formulated an equation for photon energy absorption buildup factors in the energy region 0.015–15 MeV, atomic number range $1 \leq Z \leq 92$ and for mean free path up to 40 mfp

2 Present work

We have studied the variations of the photon energy absorption buildup factors (ANSI/ANS-6.4.3, 1991). We have performed the linear/non-linear regressions/ non-linear least squares fittings. We have tried more than 100 functions such as Gaussian, sigmoidal, rational, sinusoidal, etc. that fits for a given set of data points. We have tried suitable functions such as $\alpha_1 E^{\alpha_2} + \alpha_3 E^{\alpha_4}$, $\alpha_1 + \frac{\alpha_2}{E} + \frac{\alpha_3}{E^2} + \frac{\alpha_4}{E^3}$, $\frac{1}{\left(\alpha_1 E^2 + \alpha_2 E + \alpha 3\right)}$, $\frac{\left(\alpha_1 E^{\alpha_2} + \alpha_3\right)}{\left(E^{\alpha_4} + \alpha_5\right)}$, $\left(\alpha_1 E^{\alpha_2} + \alpha_3\right)$, $\alpha_1 \exp\left(\alpha_2 E^{\alpha_3}\right) + \alpha_4$, $\alpha_1 \exp\left(\alpha_2 \left(\ln E + \alpha_3\right)^2\right) + \alpha_4$, $\frac{\alpha_1}{((E+\alpha_2)^2+1)^{\alpha_3}} + \alpha_4$, $\alpha_1 \exp\left(\frac{\alpha_2}{E} + \alpha_3 \ln E\right)$, $\alpha_1 \exp\left(\alpha_2 E\right) + \alpha_3 \exp\left(\alpha_4 E\right)$, $\alpha_1 E + \alpha_2 \exp\left(\alpha_3 E\right) + \alpha_4$, $\beta_1 E + \beta_2 + \frac{\beta_3}{E} + \beta_4 \ln E$, $\delta_1 E + \delta_2 \exp\left(\delta_3 E\right) + \delta_4$ and polynomial function $\left(\alpha_1 E^4 + \alpha_2 E^3 + \alpha_3 E^2 + \alpha_4 E + \alpha_5\right)$. After the detailed study of variations, three significant facts have been observed.

- The variation of photon EABF with energy, for a given mean free path and atomic number, is Gaussian up to Z=30 and this variation is not found to be Gaussian beyond Z=30.
- There is a systematic variation of EABF with mean free path for a given energy and atomic number.
- It is also observed that the EABF varies systematically with atomic number for a given energy and mean free path.

By considering these facts, we have proposed the following semi-empirical formula for EABF. The fitting parameters of the formula are obtained by making a linear/non-linear fit to the available data (ANSI/ANS-6.4.3, 1991). We have performed linear/polynomial regressions for the systematic data and non-linear regressions for an unsystematic data. In the non-linear optimisation methods we have tried more than 100 functions such as Gaussian, sigmoidal, rational, sinusoidal, etc. Finally, we have selected the most suitable function for the available data in the literature (ANSI/ANS-6.4.3, 1991).

2.1 EABF for 1≤Z≤29

Logarithmic energy absorption buildup factors (B_{en}) in the atomic number range 1≤Z≤29 and energy range 0.015–15MeV are represented by the following equation:

$$\log B_{en} = a \exp\left(\frac{b}{E} + c \ln E\right) \tag{1}$$

Here, a, b and c are functions of mean free path (λ) and atomic number (Z). E is photon energy in MeV. We have evaluated a, b and c using polynomial regressions and these are given below:

$$a = \lambda^3 \sum_{i=0}^{3} G_i Z^i + \lambda^2 \sum_{i=0}^{3} H_i Z^i + \lambda \sum_{i=0}^{3} J_i Z^i + \sum_{i=0}^{3} K_i Z^i \tag{1.1}$$

$$b = \lambda^3 \sum_{i=0}^{3} M_i Z^i + \lambda^2 \sum_{i=0}^{3} N_i Z^i + \lambda \sum_{i=0}^{3} P_i Z^i + \sum_{i=0}^{3} Q_i Z^i \tag{1.2}$$

$$c = \lambda^3 \sum_{i=0}^{3} R_i Z^i + \lambda^2 \sum_{i=0}^{3} S_i Z^i + \lambda \sum_{i=0}^{3} T_i Z^i + \sum_{i=0}^{3} U_i Z^i \tag{1.3}$$

The fitting parameters (G_i, H_i, J_i, K_i, M_i, N_i, P_i, Q_i, R_i, S_i, T_i and U_i) for the above equations are given in the Table 1.

Table 1 Fitting parameters for the equations (1.1), (1.2) and (1.3)

i	*Range*	*i=3*	*i=2*	*i=1*	*i=0*
G_i	18≤Z≤28	–8.85172913e-7	5.668947109e-5	–1.194394107e-3	+ 8.364081499e-3
	1≤Z≤17	6.661460796e-10	3.220850553e-9	–4.079291388e-7	7.076697074e-5
H_i	18≤Z≤28	1.560725233e-5	–1.004382223e-3	2.123833134e-2	–1.538800065e-1
	1≤Z≤17	–7.006718576e-9	–1.659107161e-6	3.427382801e-5	–5.976960209e-3
J_i	18≤Z≤28	2.580341952e-4	–1.638763069e-2	3.430377872e-1	–2.179061028
	1≤Z≤17	–1.098180993e-6	6.495581635e-5	–4.454390392e-4	1.840159198e-1
K_i	18≤Z≤28	5.28515352e-6	–1.203572036e-3	5.033541447e-2	–2.982266895e-1
	1≤Z≤17	–3.13251415e-7	–5.228198365e-5	6.916122805e-3	1.506638613e-1
M_i	18≤Z≤28	1.358446645e-7	–8.787676384e-6	1.871622247e-4	–1.316563545e-3
	1≤Z≤17	–4.518949112e-11	–4.765085547e-9	8.044773061e-8	–1.232226958e-6
N_i	18≤Z≤28	–5.206101841e-6	3.403093579e-4	–7.326782339e-3	5.217845508e-2
	1≤Z≤17	–2.389853235e-8	1.43161585e-6	–1.680645237e-5	1.107619158e-4
P_i	18≤Z≤28	4.130411998e-5	–2.789609608e-3	6.217246102e-2	–4.602969331e-1
	1≤Z≤17	–1.50881352e-7	4.032699991e-6	–6.31773973e-5	–2.046602542e-3
Q_i	18≤Z≤28	6.819859694e-5	–3.755019336e-3	5.502885528e-2	–2.954328787e-1
	1≤Z≤17	1.026157598e-6	–1.070065397e-4	–6.187007695e-3	1.050863186e-2
R_i	18≤Z≤28	9.443158697e-7	–6.075010003e-5	1.28722351e-3	–8.98825508e-3
	1≤Z≤17	9.890262387e-9	–4.045092734e-7	5.686968306e-6	–1.915274846e-5
S_i	18≤Z≤28	–5.367508189e-5	3.458839461e-3	–7.343554637e-2	5.137247671e-1
	1≤Z≤17	–3.182425156e-7	1.754956666e-5	–3.208998602e-4	1.246196323e-3
T_i	18≤Z≤28	8.687100003e-4	–5.61128629e-2	1.195195673	–8.385818251
	1≤Z≤17	4.664546039e-6	–2.792702089e-4	6.182367174e-3	–2.820262623e-2
U_i	18≤Z≤28	–3.795904652e-3	2.464030834e-1	–5.282208352	36.85262196
	1≤Z≤17	–3.794888397e-5	2.100186855e-3	–4.47077698e-2	–2.254698146e-1

2.2 EABF for 29≤Z≤45

Logarithmic energy absorption buildup factors (B_{en}) in the atomic number range 29≤Z≤45 and energy range 0.015–15MeV are represented by the following equation:

$$\log B_{en} = \varphi_1(\lambda, Z)\exp\left(\frac{\varphi_2(\lambda, Z)}{E} + \varphi_3(\lambda, Z)\ln E\right) \tag{2}$$

Here, Φ_1, Φ_2 and Φ_3 are functions of mean free path (λ) and atomic number (Z). These functions are given by the following equations:

$$\Phi_1(\lambda, Z) = -\left(-2.111233972\times10^{-3}Z + 0.1169475485\right) \lambda - 8.151610862\times10^{-3}Z + 0.6340019843 \tag{2.1}$$

$$\Phi_2(\lambda, Z) = \left(1.071978672\times10^{-4}\ Z - 1.482845899\times10^{-3}\right) \lambda + 1.429223453\times10^{-2}\ Z - 0.6536095448 \tag{2.2}$$

$$\Phi_3(\lambda, Z) = \left(2.827872308\times10^{-6}\ Z + 1.028963317\times10^{-2}\right) \lambda + 3.737112951\times10^{-2}\ Z - 1.731517885 \tag{2.3}$$

2.3.1 EABF for 46≤Z≤60 (0.15–15MeV)

Logarithmic energy absorption buildup factors (B_{en}) in the atomic number range 46≤Z≤60 and energy range 0.15–15MeV are represented by the following equation:

$$\log B_{en} = \frac{E}{\alpha_1(\lambda, Z)E^2 + \alpha_2(\lambda, Z)E + \alpha_3(\lambda, Z)} \tag{3}$$

Here, α_1, α_2 and α_3 are functions of mean free path (λ) and atomic number (Z). These functions are given by the following equations:

$$\alpha_1(\lambda, Z) = -\left(1.6602266\times10^{-3}\ Z - 9.655073576\times10^{-2}\right) \lambda - 6.588934094\times10^{-2}\ Z + 3.814702153 \tag{3.1}$$

$$\alpha_2(\lambda, Z) = \left(-3.629010801\times10^{-3}\ Z + 0.1468840778\right) \lambda + 0.13123717\ \ Z - 4.63558137 \tag{3.2}$$

$$\alpha_3(\lambda, Z) = \left(6.128943\times10^{-4}\ Z - 3.87030529\times10^{-2}\right) \lambda - 1.470753503\times10^{-2}\ Z + 1.176651602 \tag{3.3}$$

2.3.2 EABF for 46≤Z≤60 (0.015–0.15MeV)

Logarithmic energy absorption buildup factors (B_{en}) in the atomic number range 46≤Z≤60 and energy range 0.015–0.15MeV are represented by the following equation:

$$\log B_{en} = \frac{1}{\psi_1(\lambda, Z)E^2 + \psi_2(\lambda, Z)E + \psi_3(\lambda, Z)} \tag{4}$$

Here, ψ_1, ψ_2 and ψ_3 are functions of mean free path (λ) and atomic number (Z). These functions are given by the following equations:

$$\psi_1(\lambda,Z) = (15.32754387\,Z - 876.3349007)\,\lambda - 662.640706\,Z + 38208.38066 \tag{4.1}$$

$$\psi_2(\lambda,Z) = (-1.845590495\,Z + 105.065032)\,\lambda + 76.16186985\,Z - 4363.381543 \tag{4.2}$$

$$\psi_3(\lambda,Z) = \left(5.50701663\times10^{-2}\,Z - 3.223266283\right)\lambda - 2.22226919\,Z + 130.6889919 \tag{4.3}$$

2.4.1 EABF for 61≤Z≤78 (0.15–15MeV)

Logarithmic energy absorption buildup factors (B_{en}) in the atomic number range 61≤Z≤78 and energy range 0.15–15MeV are formulated as

$$\log B_{en} = \beta_1(\lambda,Z)\exp\left(\frac{\beta_2(\lambda,Z)}{E}\right) + \beta_3(\lambda,Z)\exp\left(\frac{\beta_4(\lambda,Z)}{E}\right) \tag{5}$$

Here, β_1, β_2 ,β_3 and β_4 are functions of mean free path (λ) and atomic number (Z). These functions are given by the following equations:

$$\beta_1(\lambda,Z) = \left(-1.777829029\times10^{-3}\,Z + 0.1547354802\right)\lambda + 6.135886204\times10^{-2}\,Z - 3.553570254 \tag{5.1}$$

$$\beta_2(\lambda,Z) = \left(1.826394719\times10^{-4}\,Z - 1.599685241\times10^{-2}\right)\lambda + \left(-2.027688576\times10^{-2}\,Z + 1.140218971\right) \tag{5.2}$$

$$\beta_3(\lambda,Z) = \left(-1.380799538\times10^{-3}\,Z + 0.4008981862\right)\lambda + \left(-1.974296736\times10^{-2}\,Z + 0.7376622388\right) \tag{5.3}$$

$$\beta_4(\lambda,Z) = \left(5.2097878\times10^{-3}\,Z - 0.7799795566\right)\lambda + \left(-9.942262125\times10^{-3}\,Z - 0.523408907\right) \tag{5.4}$$

2.4.2 EABF for 61≤Z≤78 (0.015–0.15MeV)

Logarithmic energy absorption buildup factors (B_{en}) in the atomic number range 61≤Z≤78 and energy range 0.015–0.15MeV are formulated as;

$$\log B_{en} = \chi_1(\lambda,Z)\exp\left(\chi_2(\lambda,Z)E^2 + \chi_3(\lambda,Z)E\right) \tag{6}$$

Here, χ_1, χ_2 and χ_3 are functions of mean free path (λ) and atomic number (Z). These functions are given by the following equations:

$$\chi_1(\lambda,Z) = \left(-9.25966706\times10^{-7}\,Z + 4.26173495\cdot10^{-6}\right)\lambda + 3.3047902\times10^{-5}\,Z + 1.26873793\times10^{-4} \tag{6.1}$$

$$\chi_2(\lambda,Z)=\left(1.862043387Z-182.3704735\right)\lambda+49.48254653\,Z-4023.728095 \tag{6.2}$$

$$\chi_3(\lambda,Z)=\left(-2.584371610^{-3}\,Z+7.288449359\right)\lambda-4.619478093\,Z+422.9920581 \tag{6.3}$$

2.5.1 EABF for 79≤Z≤92 (0.15–15MeV)

Logarithmic energy absorption buildup factors (B_{en}) in the atomic number range 79≤Z≤92 and energy range 0.15–15MeV are formulated as;

$$\log B_{en}=\delta_1(\lambda,Z)\exp\left(\frac{\delta_2(\lambda,Z)}{E}+\delta_3(\lambda,Z)\ln E\right) \tag{7}$$

Here, δ_1, δ_2 and δ_3 are functions of mean free path (λ) and atomic number (Z). These functions are given by the following equations:

$$\delta_1(\lambda,Z)=\left(-1.235400727\times10^{-3}\,Z+0.1124518895\right)\lambda+\left(-3.83505956\times10^{-3}\,Z+0.5362862617\right) \tag{7.1}$$

$$\delta_2(\lambda,Z)=\left(1.809207489\times10^{-3}\,Z-0.143145422\right)\lambda+\left(5.481956141\times10^{-3}\,Z-0.4495204036\right) \tag{7.2}$$

$$\delta_3(\lambda,Z)=\left(1.438477261\times10^{-3}Z-9.857595326\times10^{-2}\right)\lambda+\left(4.021971227\times10^{-3}Z-0.3491808228\right) \tag{7.3}$$

2.5.2 EABF for 79≤Z≤92 0.015-0.15MeV

Logarithmic energy absorption buildup factors (B_{en}) in the atomic number range 79≤Z≤92 and energy range 0.015–0.15MeV are formulated as;

$$\log B_{en}=\frac{1}{\eta_1(\lambda,Z)E^3+\eta_2(\lambda,Z)E^2+\eta_3(\lambda,Z)E+\eta_4(\lambda,Z)} \tag{8}$$

Here, η_1, η_2, η_3 and η_4 are functions of mean free path (λ) and atomic number (Z). These functions are given by the following equations:

$$\eta_1(\lambda,Z)=\left(4.87208971\,Z-407.3809183\right)\lambda-218.8679639\,Z+17816.13916 \tag{8.1}$$

$$\eta_2(\lambda,Z)=\left(-18.39576711\,Z+1428.862113\right)\lambda+761.7686238\,Z-58876.77629 \tag{8.2}$$

$$\eta_3(\lambda,Z)=\left(4.800142482\,Z-374.6446991\right)\lambda-198.7193849\,Z+15466.86024 \tag{8.3}$$

$$\eta_4(\lambda,Z)=\left(-0.3219200222\,Z+25.20157399\right)\lambda+13.34597215\,Z-1043.101492 \tag{8.4}$$

3 Results and discussion

The formulated semi-empirical equations for photon EABF of atomic number region $1 \leq Z \leq 92$ and in the energy region 0.015–15 MeV up to 40 mean free paths are represented in the equations (1)–(8). To validate the above formulae, we have evaluated EABF for elements using this formulae and compared them with the data available in the literature (ANSI/ANS-6.4.3, 1991). The comparison of evaluated EABF using present formulae with that of GP fitting method for elements is as shown in the Figures 1–3. From these figures, it is clear that the photon EABF evaluated by the present formulae agree well with that of the GP fitting method. So the present formulae can be used to compute the photon EABF for elements of atomic number region $1 \leq Z \leq 92$ and in the energy region 0.015–15 MeV up to 40 mean free paths. In this method photon EABF can be computed without the knowledge of the GP fitting parameters.

We can also extend these formulae to any compounds/mixtures/biological samples by using the concept of equivalent atomic number (Z_{eq}). The equation for equivalent atomic number (Z_{eq}) was given by the previous researchers (Sidhu et al., 2000):

$$Z_{eq} = \frac{Z_1 \left(\log R_2 - \log R\right) + Z_2 \left(\log R - \log R_1\right)}{\left(\log R_2 - \log R_1\right)} \tag{9}$$

where Z_1 and Z_2 are the elemental atomic numbers corresponding to the ratios (μ_{comp}/μ_{tot}) R_1 and R_2, respectively, and R is the ratio for the chosen compounds/mixtures/biological samples at particular energy. μ_{comp} and μ_{tot} are the attenuation coefficients corresponding to Compton scattering and total interaction process respectively. EABF values for compounds/mixtures/biological samples are computed by substituting $Z=Z_{eq}$ in the corresponding equations (1)–(8). For instance, if Z_{eq} for adipose tissue is 4.5, then EABF for adipose tissue for different energies (0.015–15MeV) up to 40 mfp are computed by substituting $Z=4.5$ in the equation (1). In this way, these formulated equations may also be used to compute EABF for any compounds/mixtures/biological samples. This semi-empirical formula finds importance in the calculations of buildup factors of any materials which is required for radiation shielding, nuclear engineering, radiotherapy and nuclear medicine.

Figure 1 The comparison of evaluated EABF using present formulae with that of GP fitting method for elements

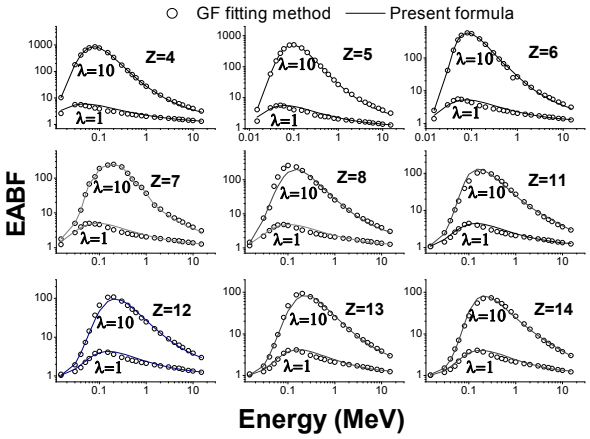


Figure 2 The comparison of evaluated EABF using present formulae with that of GP fitting method for elements

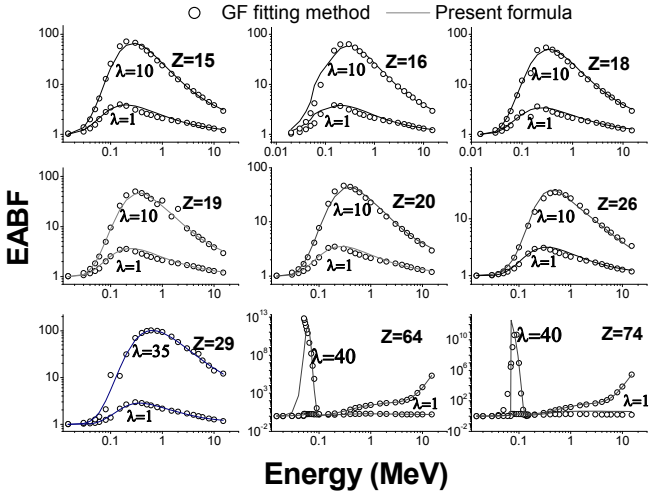
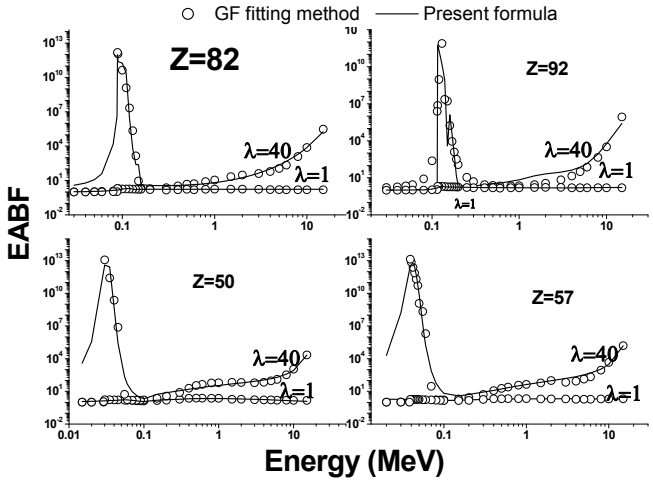


Figure 3 The comparison of evaluated EABF using present formulae with that of GP fitting method for elements



4 Conclusion

We have formulated a simple semi-empirical formulae for photon energy absorption buildup factors in the energy region 0.015–15 MeV, atomic number range $1 \leq Z \leq 92$ and for mean free path up to 40 mfp. The results produced by the present formulae agree well with the data available in the literature (ANSI/ANS-6.4.3, 1991). This semi-empirical formula may be extending to any compounds/mixtures/biological samples.

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