# SEMI-EMPIRICAL RELATIONSHIP FOR THE ENERGY ABSORPTION BUILDUP FACTOR IN SOME BIOLOGICAL SAMPLES

by

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Energy absorption buildup factors in the energy range of 0.2 MeV to 2 MeV using a geometric progression fitting approximation in some selected essential amino acids, fatty acids and carbohydrate molecules have been obtained. A semi empirical relation-ship describing energy absorption buildup factors as a function of penetration depth, Compton scattering and energy absorption cross-section is used. This semi empirical method was defined in an earlier work on water and soft tissue by one of the present authors. We used this method for the calculating energy absorption buildup factor in biological samples. The results are compared with the energy absorption buildup factors data of the geometric progression fitting methods has been observed, so that average deviation is less than 2 % for all samples.

Key words: buildup factor, GP fitting, biological sample, semi empirical relationship

## INTRODUCTION

The buildup factor is one of the important properties of a material used for beam collimation, tissue compensation or radiation shielding and protection. It directly affects the absorbed dose quantity and hence, correct dose delivery to a tumor is not possible without the knowledge of the buildup factor of the material for tissue compensation purposes. For narrow beam geometry B = 1 exactly, and for broad beam geometry B > 1. In narrow beam geometry, ideally there is no scattered or secondary radiation to detect, so there is no buildup factor contributing to the detected radiation. However, broad beam geometry will usually produce some type of secondary scattered radiation which depends on the geometry and components involved. The value of *B* is a function of radiation type and energy, attenuating medium and thickness, geometry, and measured quantity [1].

Up to now, studies about energy absorption buildup factors (EABF) in biological samples have been widely made using the well-known methods such as, the geometric progression (GP) fitting method, generalized feed-forward neural network (GFFNN), and Monte Carlo based codes [2-11].

Recently, Sardari and Baradaran [12] developed a new relationship estimating the buildup factor as a function of penetration depth, Compton scattering, and energy absorption cross-sections. In another work Sardari and Kurudirek [13] developed this semi empirical equation approach to the data obtained through a five parameter GP fitting method to the EABF for soft tissue, water, and hydrogen, carbon, nitrogen and oxygen based dosimetric materials.

Recently Kurudirek and Ozdemir [14] estimated the energy absorption and exposure buildup factors by using the G-P fitting method for some biological molecules such as amino acids, fatty acids and carbohydrates in the energy region 0.015-15 MeV up to penetration depths of 40 mfp<sup>\*\*</sup>. Meanwhile, the chemical composition data of these biological molecules were taken from their study. In the present study, we have applied the semi-empirical relationship to calculate the energy absorption buildup factor data for some biological molecules such as mustard oil, glucose, mannitol, sucrose, ribose and valine.

#### MATERIALS AND METHODS

## **GP** fitting method

To calculate the buildup factors, the G-P fitting parameters were obtained by the method of interpolation from the equivalent atomic number ( $Z_{eq}$ ). Computations are illustrated step by step as follows:

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<sup>\*\*</sup> mean free path

B(E r) = 1 (h - 1)r

- (a) calculation of the equivalent atomic number,  $Z_{eq}$ ,
- (b) calculation of geometric progression (G-P) fitting parameters. and
- (c) calculation of energy absorption and exposure buildup factors.

In the first step, the equivalent atomic number,  $Z_{ea}$ , for a particular material has been calculated by matching the ratio ( $\mu \rho$ ) <sub>Compton</sub> /( $\mu \rho$ ) <sub>total</sub>, of that material at a specific energy with the corresponding ratio of an element at the same energy.

Thus, firstly the Compton partial mass attenuation coefficient,  $(\mu \rho)_{\text{Compton}}$ , and the total mass attenuation coefficients,  $(\mu \rho)_{total}$ , were obtained for the elements of Z = 4-40 and for the chosen materials in the energy region 0.015 to 15 MeV, using the WinXCom computer program [15, 16] that was initially developed as XCOM [17]. When the ratio ( $\mu \rho$ ) <sub>Compton</sub>  $/(\mu \rho)$  total lies between two successive ratios of elements, the following formula is employed for the interpolation of  $Z_{eq}$  [2]

$$Z_{\rm eq} = \frac{Z_1(\log R_2 - \log R) - Z_2(\log R - \log R_1)}{\log R_2 - \log R_1} (1)$$

where  $Z_1$  and  $Z_2$  are the elemental atomic numbers corresponding to the ratios  $R_1$  and  $R_2$ , respectively, and Ris the ratio for the soft tissue at the specific energy.

In the second step, to calculate the G-P fitting parameters, a similar interpolation procedure was adopted as in the case of an equivalent atomic number. The G-P fitting parameters for elements were taken from the ANSI/ANS-6.4.3 [18] standard reference database, which provides the G-P fitting parameters for elements, from beryllium to iron in the energy region 0.015-15 MeV up to a depth of 40 mfp. G-P fitting buildup factor coefficients of the materials under consideration were interpolated according to the given formula

$$P = \frac{P_1 (\log Z_2 - \log Z_{eq}) - P_2 (\log Z_{eq} - \log Z_1)}{\log Z_2 - \log Z_1}$$
(2)

where P is the G-P fitting function coefficient corresponding to  $Z_{eq}$ ,  $P_1$  and  $P_2$  are the values of G-P fitting function coefficients corresponding to the elemental atomic numbers  $Z_1$  and  $Z_2$ , at a given energy, respectively, where as  $Z_{eq}$  is the equivalent atomic number of the chosen material at the given energy.

In the final step, the computed G-P fitting parameters  $(b, c, a, X_k, and d)$  are used to compute the EABF of these amino acids in the energies 0.015-15 MeV and penetration depths up to 40 mfp with the help of the G-P fitting formula, as given by the equations

$$B(E,x) = 1 - \frac{(b-1)(K^X - 1)}{K - 1}, \quad \text{for } K = 1$$
 (3)

$$B(E,x) \quad 1 \quad (b \quad 1)x, \quad \text{for } K \quad 1 \qquad (4)$$
  
where  
$$K(E,x) \quad cx^{a}$$

for K 1

$$d \frac{\tanh(x/X_{k} \ 2) \ \tanh(2)}{1 \ \tanh(2)}, \quad \text{for } (x) \ \text{mfp} (5)$$

and E is the incident photon energy, x – the penetration depth in mfp, a, b, c, d, and  $X_k$  are the G-P fitting parameters and b is the value of the buildup factor at 1 mfp. The parameter K represents photon dose multiplication and a change in the shape of the spectrum [9]. The GP fitting values of buildup factors for these amino acids was taken from the previous study for comparison [14].

#### Semi empirical approach

The atomic mixture of mustard oil, glucose, mannitol, sucrose, ribose, and valine is C22H42O2,  $C_6H_{12}O_6, C_6H_{14}O_6, C_{12}H_{22}O_{11}, C_5H_{10}O_5, and C_5H_{11}O_2N,$ respectively. Using the data along with the microscopic cross-sections for energy absorption ( $\sigma_a$ ) and Compton scattering ( $\sigma_s$ ), the macroscopic cross-sections in amino acids containing H, C, O, and N are obtained using the equations

$${}_{\mathrm{a}} \quad N_{\mathrm{H}}\sigma_{s}^{H} \quad N_{\mathrm{O}}\sigma_{s}^{O} \quad N_{\mathrm{C}}\sigma_{s}^{C} \quad N_{\mathrm{N}}\sigma_{s}^{N} \quad (6)$$

$$_{\rm s} N_{\rm H} \sigma_a^H = N_{\rm O} \sigma_a^O = N_{\rm C} \sigma_a^C = N_{\rm N} \sigma_a^N$$
 (7)

The microscopic cross-sections data are shown in tab. 1. The macroscopic scattering and absorption cross-section and ratio of macroscopic scattering to absorption cross-section  $(\Sigma_s / \Sigma_a)$  are shown in tab. 2.

Table 1. Scattering and energy absorption cross-sections for hydrogen, oxygen, nitrogen, and carbon

E [MeV]	$\Sigma_s^H  [\mathrm{cm}^{-1}]$	$\Sigma_a^H  [\mathrm{cm}^{-1}]$	$\Sigma_s^O$ [cm <sup>-1</sup> ]	$\Sigma_a^O$ [cm <sup>-1</sup> ]	$\Sigma_s^N$ [cm <sup>-1</sup> ]	$\Sigma_a^N$ [cm <sup>-1</sup> ]	$\Sigma_s^C$ [cm <sup>-1</sup> ]	$\Sigma_a^C$ [cm <sup>-1</sup> ]
0.2	0.319	0.0879	2.5	0.711	0.223	0.619	1.91	0.539
0.3	0.258	0.0953	1.814	0.668	1.56	0.572	2.078	0.764
0.4	0.219	0.098	1.527	0.687	1.315	0.589	1.751	0.783
0.5	0.19	0.099	1.527	0.789	1.335	0.69	1.143	0.592
0.6	0.169	0.098	1.184	0.688	1.012	0.59	1.355	0.786
0.8	0.139	0.096	0.973	0.672	0.837	0.576	1.122	0.768
1	0.118	0.093	0.947	0.743	0.83	0.65	0.71	0.557
2	0.069	0.078	0.549	0.632	0.481	0.553	0.412	0.472

	Mustard oil			Glucose			Mannitol		
E [MeV]	$\Sigma_{\rm s}  [{\rm cm}^{-1}]$	$\Sigma_{\rm a}  [{\rm cm}^{-1}]$	$\Sigma_{\rm s}/\Sigma_{\rm a}$	$\Sigma_{\rm s}  [{\rm cm}^{-1}]$	$\Sigma_{\rm a}  [{\rm cm}^{-1}]$	$\Sigma_{\rm s}/\Sigma_{\rm a}$	$\Sigma_{\rm s}  [{\rm cm}^{-1}]$	$\Sigma_{\rm a}  [{\rm cm}^{-1}]$	$\Sigma_{\rm s}/\Sigma_{\rm a}$
0.2	60.41	16.97	3.55	30.28	8.55	3.54	30.92	8.73	3.54
0.3	60.18	22.14	2.71	26.44	9.73	2.71	26.96	9.92	2.71
0.4	50.77	22.71	2.23	22.29	9.99	2.23	22.73	10.19	2.23
0.5	36.18	18.76	1.92	18.3	9.47	1.93	18.68	9.67	1.93
0.6	39.27	22.78	1.72	17.26	10.02	1.72	17.6	10.21	1.72
0.8	32.46	22.27	1.45	14.23	9.79	1.45	14.51	9.98	1.45
1	22.47	17.64	1.27	11.35	8.91	1.27	11.59	9.10	1.27
2	13.06	14.92	0.87	6.59	7.56	0.87	6.73	7.71	0.87
	Sucrose		Ribose			Valine			
E [MeV]	$\Sigma_{\rm s} [{\rm cm}^{-1}]$	$\Sigma_{\rm a}  [{\rm cm}^{-1}]$	$\Sigma_{\rm s}/\Sigma_{\rm a}$	$\Sigma_{\rm s} [{\rm cm}^{-1}]$	$\Sigma_{\rm a}  [{\rm cm}^{-1}]$	$\Sigma_{\rm s}/\Sigma_{\rm a}$	$\Sigma_{\rm s} [{\rm cm}^{-1}]$	$\Sigma_{\rm a}  [{\rm cm}^{-1}]$	$\Sigma_{\rm s}/\Sigma_{\rm a}$
0.2	57.43	16.22	3.54	25.24	7.129	3.54	18.28	5.70	3.20
0.3	50.56	18.61	2.7	22.04	8.113	2.71	18.41	6.77	2.71
0.4	42.62	19.1	2.23	18.58	8.33	2.23	15.53	6.95	2.23
0.5	34.69	17.961	1.93	15.25	7.895	1.93	12.19	6.31	1.93
0.6	33	19.15	1.72	14.38	8.35	1.72	12.01	6.97	1.72
0.8	27.22	18.72	1.45	11.86	8.16	1.45	9.92	6.81	1.45
1	21.53	16.9	1.27	9.46	7.43	1.27	7.57	5.94	1.27
2	12.5	14.33	0.87	5.49	6.3	0.87	4.39	5.03	0.87

Table 2. Ratio of scattering to absorption cross-section for mustard oil, glucose, mannitol, sucrose, ribose, and valine

The following semi-empirical relationship was used to describe the variations of buildup factor as function of energy absorption cross-sections and penetration depth r

$$B = 1 \quad a\mu r \frac{\Sigma_s}{\Sigma_a} \tag{8}$$

where a and b are parameters to be found so that the results of eq. 1 fit to the data obtained from the GP fitting method. The following relationship was defined for OR-IGIN software with a given set of B and X as input data

$$B \quad (1 \quad aX)^b \tag{9}$$

For each set of data at specific photon energies, ORIGIN computed the best quantity for a and b parameters. The values of these parameters are listed in tab. 3 for these amino acids in the energy range of 0.2 MeV-2 MeV.

For detailed explanations on the semi-empirical relation and microscopic cross-sections of H, C, O, and N used in this study, we may refer to the previous study in which the use of a semi empirical relation is explained in detail [12].

## **RESULTS AND DISCUSION**

The computed buildup factor data obtained by the GP fitting method and eq. (8) are collected in tab. 4.

The relative differences in buildup factors between the semi empirical and GP fitting method are shown in tab. 5. It has been observed that the differences decrease with the increase in energy and penetration depth, so in 2 MeV the differences are very low (0.7). At 0.5 MeV the difference in some samples is partly high, so that the average difference for glucose is about 8 % and for value is about 4 %. At 2 MeV except for glucose (its average difference is 7 %); the average difference is less than 1.5 % and at 10 MeV the average difference is less than 0.5 % for all samples. It has been observed, that there is good agreement between semi empirical and GP fitting methods so that the average difference is less than 2 % for these samples.

These results indicate that ribose has the minimum differences in all energies and penetration depths while the maximum differences are for glucose.

## CONCLUSION

In the present study, a semi-empirical relationship was applied to the energy absorption buildup factor data obtained from the GP fitting method. The results are quite satisfactory for mustard oil, glucose, mannitol, sucrose, ribose and valine. It was concluded that for lower penetration depths (<10 mfp) and photon ener-

Table 3. Parameters a and b for the energy absorption buildup factor in eq. (8) for various energies

	0.2 []	MeV]	0.5 []	MeV]	2 [MeV]		
	а	b	а	b	а	b	
Mustard oil	0.11	3.29	0.23	2.43	0.68	1.31	
Glucose	0.14	2.7	0.23	2.3	0.68	1.31	
Mannitol	0.11	3.31	0.23	2.42	0.68	1.31	
Sucrose	0.12	3.2	0.23	2.42	0.68	1.31	
Ribose	0.11	3.32	0.23	2.43	0.68	1.31	
Valine	0.11	3.47	0.23	2.43	0.68	1.31	

<i>r</i> (mfp)	Mustard oil	Glucose	Mannitol	Sucrose	Ribose	Valine		
GP fitting								
1	2 20	2.50	0.2 Mev	2.24	2.22	2 27		
2	3.29	5.39	3.23	3.34	3.23	3.27		
2	7.84	/.8/	7.78	7.92	7.70	7.82		
4	26.54	22.14	26.69	20.33	26.73	20.0		
/	93.30	61.83	95.6	90.44	96.2	94.2		
10	234.4	129.6	243.5	222.8	246	237.8		
0.5 MeV								
	2.46	2.53	2.45	2.46	2.45	2.45		
2	4.83	4.86	4.83	4.83	4.83	4.83		
4	12.54	11.89	12.58	12.5	12.59	12.56		
10	32.86	29.07	33.1	32.56	33.16	32.94		
10	65.15	54.95	65.92	64.2	66.13	65.43		
			2 MeV					
1	1.84	1.83	1.84	1.84	1.84	1.83		
2	2.8	2.79	2.8	2.79	2.8	2.79		
4	4.96	4.94	4.96	4.96	4.96	4.95		
7	8.66	8.63	8.67	8.66	8.67	8.65		
10	12.77	12.72	12.78	12.76	12.78	12.73		
			Eq. 8					
	T		0.2 MeV					
1	3.21	3.04	3.22	3.21	3.23	3		
2	7.59	6.67	7.64	7.55	7.68	7.21		
4	26.38	20.11	26.69	25.84	26.95	25.21		
7	94.28	60.45	96	90.35	97.35	92.42		
10	235.6	131.8	241.13	221.6	245.2	237.3		
			0.5 MeV					
1	2.5	2.37	2.48	2.48	2.5	2.5		
2	4.86	4.45	4.81	4.82	4.86	4.86		
4	12.57	10.95	12.40	12.4	12.6	12.59		
7	32.93	27.19	32.29	32.3	33.03	32.99		
10	65.54	52.09	64	64.02	65.74	65.66		
2 MeV								
1	1.85	1.84	1.84	1.84	1.84	1.84		
2	2.81	2.8	2.8	2.8	2.8	2.8		
4	4.97	4.95	4.95	4.95	4.95	4.96		
7	8.67	8.64	8.65	8.64	8.64	8.66		
10	12.81	12.76	12.77	12.76	12.76	12.78		

Table 4. Energy absorption buildup factor data obtained by different methods for mustard oil, glucose, mannitol, sucrose, ribose, and valine

gies lower than 2 MeV, the presented semi-empirical approximation can be used as a safe tool to estimate buildup factors for gamma and X-rays in these biological samples.

#### **AUTHORS' CONTRIBUTIONS**

Computational work was carried out by D. Salehi, theoretical work by D. Sardari. Data collection and comparison by D. Salehi and M. S. Jozani. The whole manuscript was edited by D. Sardari and reviewed by all the authors.

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r (mfp)	Mustard oil	Glucose	Mannitol	Sucrose	Ribose	Valine			
0.2 MeV									
1	2.4	15.4	0.7	3.9	0.08	5.8			
2	3.3	15.2	1.8	4.6	0.9	7.8			
4	0.6	9.1	0	1.8	0.8	5.2			
7	0.9	2.2	0.4	0.09	1.1	1.8			
10	0.4	1.6	0.9	0.5	0.3	0.2			
	0.5 MeV								
1	1.6	6.1	1.2	1.1	1.8	1.7			
2	0.4	8.2	0.3	0.2	0.6	0.6			
4	0.2	7.9	1.4	0.7	0.1	0.2			
7	0.2	6.4	2.4	0.7	0.4	0.1			
10	0.5	5.2	2.9	0.2	0.58	0.3			
			2 MeV						
1	0.5	0.5	0.3	0.4	0.3	0.7			
2	0.3	0.3	0.1	0.1	0.1	0.4			
4	0.2	0.2	0.08	0.04	0.1	0.2			
7	0.1	0.1	0.2	0.16	0.2	0.1			
10	0.3	0.3	0.07	0	0.1	0.3			

Table 5. Relative difference [%] between the buildup factor values for biological samples obtained through eq. 8. and GP fitting approximation

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## ПОЛУЕМПИРИЈСКА РЕЛАЦИЈА ЗА ЕНЕРГЕТСКИ ФАКТОР НАГОМИЛАВАЊА У НЕКИМ БИОЛОШКИМ УЗОРЦИМА

Одређени су енергетски фактори нагомилавања у опсегу енергија од 0.2 MeV до 2 MeV израчунати фитовањем геометријском прогресијом у изабраним амино киселинама, масним киселинама и карбохидратним молекулима. Коришћена је полуемпиријска релација која описује енергетски фактор нагомилавања као функцију дубине продирања и ефикасних пресека за Комптоново расејање и енергетску апсорпцију. Овај полуемпиријски метод већ је дефинисан за воду и меко ткиво у претходном раду једног од аутора. Искористили смо овај метод за прорачун енергетског фактора нагомилавања у биолошким узорцима. Резултати су упоређени са подацима добијени методом фитовања геометријском прогресијом. Уочено је добро слагање резултата полуемпиријског метода и фитовања геометријском прогресијом, тако да је средња девијација мања од 2 % за све узорке.

Кључне речи: факшор нагомилавања, фишовање геомешријском прогресијом, биолошки узорак, полуемпиријска релација