Research Article

Determination of Effective Atomic Numbers Using Different Methods for Some Low-Z Materials

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Received 18 April 2014; Revised 4 July 2014; Accepted 9 July 2014; Published 7 August 2014

Academic Editor: Hasan Mahmood Khan

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In the present work, different methods were used to determine the effective atomic numbers of some low-Z materials, namely, polyethylene (PE), polystyrene (PS), polypropylene (PP), Perspex (PX), polycarbonate (PC), nylon 6-6 (PA-6), plaster of Paris (POP), and TH/L2. These methods are the direct method, the interpolation method, Auto- Z_{eff} software, and single value XMuDat computer program. Some of the results obtained were compared with experimental data wherever possible. It can be concluded from this work that the effective atomic numbers calculated with the direct, the interpolation and Auto- Z_{eff} methods demonstrate a good agreement in Compton scattering and pair production energy regions. A large difference in the effective atomic numbers calculated by the direct and the interpolation methods of low-Z materials was also observed in photoelectric and pair production regions. It was determined that PE, PS, PX, and PA-6 were equivalent to adipose and muscle; POP was equivalent to cortical bone; TH/L2 was equivalent to thyroid tissue; PP was equivalent to yellow bone marrow and adipose tissues; PC was equivalent to spongiosa.

1. Introduction

Simulation of radiation dose distribution in human organs and tissues is possible by tissue equivalent materials. ICRU report 44 [1] describes various types of tissue substitutes for human organs and tissues. Tissue substitutes are being used for phantom, medical applications, radiology, nuclear engineering, health physics, radiation physics, radiation dosimetry, radiation protection, and space research. The effective atomic number is photon interaction parameter which is used for dosimetric properties. The effective atomic numbers can be calculated using different methods such as the direct method, the interpolation method, Auto- Z_{eff} software, and single value XMuDat computer program. Many researchers have made extensive effective atomic numbers studies on a variety of materials such as gaseous mixtures [2], dosimetric materials [3–5], alloys [6–9], semiconductors [10, 11], building materials [12], glasses [13, 14], soils [15, 16], amino acids [17], fatty acids [18], minerals [19], and biological samples [20, 21].

In this study, the effective atomic numbers for low-Z materials have been determined using the direct, the interpolation, Auto- Z_{eff} , and XMuDat methods. The theoretical results were compared with experimental data wherever possible. This study should be useful for readily available effective atomic numbers of the low-Z materials for choice of appropriate computational method.

2. Calculation Methods

Mass attenuation coefficient and attenuation cross-section data are available in photon energy range of 1 keV to 100 GeV in the form XCOM program [22] which has been transformed to windows operating system software WinXCom [23]. The atomic number and atomic masses of the elements have been taken from recent report on atomic weight of elements 2011, IUPAC [24]. The effective atomic numbers are derived by calculation of the mass attenuation coefficients and atomic cross-sections of the elements of compound/mixture. The elemental compositions of the low-Z materials used in this

TABLE 1: Elemental compositions of the low-Z materials.

Tissue substitute	Element weight (%)									
	H	C	N	O	Na	P	S	Cl	K	Ca
Polyethylene (PE)	14.37	85.63	—	—	—	—	—	—	—	—
Polystyrene (PS)	11.18	88.82	—	—	—	—	—	—	—	—
Polypropylene (PP)	14.37	85.63	—	—	—	—	—	—	—	—
Perspex (PX)	8.050	59.98	—	31.96	—	—	—	—	—	—
Polycarbonate (PC)	7.060	78.92	—	14.02	—	—	—	—	—	—
nylon 6-6 (PA-6)	9.800	63.68	12.38	14.14	—	—	—	—	—	—
Plaster of Paris (POP)	2.300	—	—	55.80	—	—	18.6	—	—	23.3
TH/L2	10.00	13.60	2.200	73.50	0.2	0.1	—	0.1	0.2	—

study are given in Table 1. The calculation methods for the effective atomic numbers of the low-Z materials are described in the following subsections.

2.1. Auto- Z_{eff} Method. Auto- Z_{eff} method is user-friendly software in visual basic for rapid computation of the average atomic numbers and spectral-weighted mean atomic numbers. The Auto- Z_{eff} surpasses dubious power-law approach. In this method, effective atomic number is determined via exploitation of the smooth correlation between atomic cross-section and atomic number. A matrix of cross-sections was constructed spanning atomic number $Z = 1 - 100$ for photon energies ranging between 10 keV and 1 GeV and the cross-sections of polyelemental media are calculated by linear additivity. The cross-sectional values are constructed with the cross-section matrix as a function of Z , and an effective atomic number is obtained by the interpolation of Z values between adjacent cross-section data [25].

2.2. Direct Method. Calculation of the effective atomic numbers $Z_{\text{eff,PI}}$ of the low-Z materials for total photon interaction was carried out by using practical formula [26]. The formula is given below:

$$Z_{\text{eff,PI}} = \frac{\sum_i f_i A_i (\mu/\rho)_i}{\sum_j (f_j A_j / Z_j) (\mu/\rho)_j}, \quad (1)$$

where f_i is molar fraction in the mixture/compound, μ is linear attenuation coefficient, ρ is density, μ/ρ is mass attenuation coefficient, A is atomic weight, Z is atomic number, and the ratio, A/Z , between the atomic mass and the atomic number is approximately constant.

2.3. Interpolation Method. Mass attenuation coefficient values $\mu_m (= \mu/\rho)$ are derived for the selected low-Z materials using the mixture rule: $(\mu/\rho)_{\text{material}} = \sum_i^n w_i (\mu/\rho)_i$, where w_i is the proportion by weight and $(\mu/\rho)_i$ is mass attenuation coefficient of the i th element tabulated in XCOM [22] software or WinXCom [23] software. The quantity w_i is given by $w_i = n_i A_i / \sum_j^n n_j A_j$ with condition $\sum_i^n w_i = 1$, where A_i is the atomic weight of the i th element and n_i is the number of formula units in the compounds.

The attenuation cross-section (σ) values of the composite material are computed by using the following relation:

$$\sigma = \frac{(\mu_m)}{N \sum_i (w_i / A_i)} \left(\frac{\text{barn}}{\text{molecule}} \right), \quad (2)$$

where $N = 6.023 \times 10^{23}$ is Avogadro's number in atom g^{-1} , w_i is weight fraction of the i th element in a molecule of the tissue substitutes, and A_i is the atomic weight of the i th element in a molecule. w_i and A_i are both dimensionless quantities.

The equivalent atomic numbers using the logarithmic interpolation formula is given as follows:

$$Z_{\text{eq}} = \frac{Z_1 (\log \sigma_2 - \log \sigma) + Z_2 (\log \sigma - \log \sigma_1)}{\log \sigma_2 - \log \sigma_1}, \quad (3)$$

where σ_1 and σ_2 are elemental atomic cross-section (barn/atom) for atomic numbers of elements corresponding to Z_1 and Z_2 , and σ is atomic cross-section of the composite materials lying between the σ_1 and σ_2 .

2.4. XMuDat Method. XMuDat computer program is able to produce a single value effective atomic number for compounds [27]. The XMuDat uses the following formula for calculation of the effective atomic number:

$$Z_{\text{eff,XMuDat}} = \left(\sum_i \alpha_i Z_i^{m-1} \right)^{1/(m-1)}, \quad (4)$$

where α_i is the fractional number of the electrons of the i th element and m is a constant between 3 and 5. It is preferred that m is set to 3.6 for materials with $Z_{\text{eff}} < 6$ and 4.1 for materials with $Z_{\text{eff}} > 6$ [28].

3. Results and Discussion

The variation of the effective atomic numbers of the low-Z materials with photon energy is shown in Figures 1(a), 1(b), 1(c), 1(d), 1(e), 1(f), 1(g), and 1(h). The effective atomic numbers below 10 keV were not compared due to large uncertainty ($\pm 25\%$) in Auto- Z_{eff} [25]. From Figures 1(a), 1(b), 1(c), 1(d), 1(e), 1(f), 1(g), and 1(h) it is clearly seen that the effective atomic numbers calculated by Auto- Z_{eff} , the direct, and the interpolation methods are in very good

TABLE 2: (a) Effective atomic numbers calculated with the direct and the interpolation methods for PE, PS, and PP with experimental data. (b) Effective atomic numbers calculated with the direct and the interpolation methods for PX, PC, and PA-6 with experimental data.

(a)

Energy (MeV)	PE			PS			PP		
	$Z_{\text{eff,PI}}$	Z_{eq}	a	$Z_{\text{eff,PI}}$	Z_{eq}	b	$Z_{\text{eff,PI}}$	Z_{eq}	b
0.013	4.688	4.462	4.5	4.947	4.702	—	4.688	4.460	—
0.017	4.027	4.191	4.1	4.359	4.479	—	4.027	4.188	—
0.022	3.515	3.813	3.8	3.872	4.163	—	3.515	3.810	—
0.026	3.234	3.504	—	3.593	3.877	—	3.234	3.500	—
0.032	3.017	3.205	3.1	3.371	3.594	—	3.017	3.201	—
0.033	2.988	3.160	—	3.340	3.551	—	2.988	3.155	—
0.044	2.823	2.913	2.9	3.167	3.284	—	2.823	2.910	—
0.054	2.762	2.833	—	3.102	3.175	—	2.762	2.829	—
0.060	2.742	2.806	—	3.081	3.138	2.98	2.742	2.803	2.64
0.081	2.703	2.756	—	3.040	3.067	—	2.704	2.753	—
0.123	2.681	2.727	—	3.016	3.025	—	2.681	2.723	—
0.279	2.670	2.713	—	3.004	3.005	—	2.670	2.709	—
0.356	2.669	2.712	—	3.002	3.003	—	2.669	2.708	—
0.511	2.668	2.711	—	3.001	3.002	3.00	2.668	2.707	2.67
0.662	2.667	2.710	—	3.001	3.001	3.00	2.667	2.707	2.66
1.115	2.667	2.711	—	3.001	3.002	—	2.667	2.708	—
1.173	2.667	2.710	—	3.001	3.001	3.00	2.667	2.707	2.66
1.274	2.667	2.710	—	3.001	3.000	3.00	2.667	2.706	2.66
1.333	2.668	2.710	—	3.001	3.001	3.00	2.668	2.706	2.66

^a Values have been reported by Parthasaradhi et al. [29]. ^b Values have been reported by Kucuk et al. [30].

(b)

Energy (MeV)	PX						PC			PA-6		
	$Z_{\text{eff,PI}}$	Z_{eq}	c	d	a	e	$Z_{\text{eff,PI}}$	Z_{eq}	a	$Z_{\text{eff,PI}}$	Z_{eq}	c
0.013	6.210	5.606	—	—	5.6	—	5.789	5.374	5.8	5.707	5.221	—
0.017	5.615	5.453	—	—	5.4	—	5.281	5.226	5.5	5.072	5.035	—
0.022	5.014	5.201	—	—	5.2	—	4.788	4.996	5.3	4.483	4.738	—
0.026	4.612	4.931	—	4.822	—	—	4.469	4.757	—	4.115	4.442	—
0.032	4.258	4.580	—	—	4.6	—	4.195	4.468	4.8	3.806	4.088	—
0.033	4.206	4.518	—	4.399	—	—	4.156	4.418	—	3.762	4.028	—
0.044	3.903	4.088	—	—	—	—	3.926	4.077	4.4	3.509	3.677	—
0.054	3.785	3.906	—	—	—	3.53	3.837	3.935	—	3.413	3.531	—
0.060	3.745	3.848	—	3.823	—	—	3.808	3.890	—	3.381	3.481	—
0.081	3.669	3.736	—	—	—	3.43	3.751	3.803	—	3.320	3.385	—
0.123	3.627	3.673	—	—	—	3.62	3.718	3.755	—	3.286	3.330	—
0.279	3.606	3.641	3.6	—	—	—	3.702	3.729	—	3.268	3.303	3.1
0.356	3.604	3.640	—	—	—	3.71	3.700	3.729	—	3.266	3.301	—
0.511	3.602	3.637	—	—	—	3.67	3.699	3.726	—	3.265	3.299	—
0.662	3.601	3.636	3.4	—	—	3.52	3.698	3.726	—	3.264	3.298	2.9
1.115	3.601	3.637	3.3	—	—	—	3.698	3.727	—	3.264	3.299	2.9
1.173	3.601	3.636	—	—	—	3.61	3.698	3.726	—	3.264	3.298	—
1.274	3.601	3.635	—	—	—	3.56	3.698	3.725	—	3.264	3.297	—
1.333	3.601	3.635	—	—	—	3.57	3.698	3.725	—	3.264	3.297	—

^a Values have been reported by Parthasaradhi et al. [29]. ^c Values have been reported by Kumar et al. [31]. ^d Values have been reported by Vijayakumar et al. [32]. ^e Values have been reported by El-Kateb and Abdul-Hamid [33].

FIGURE 1: The effective atomic numbers of low-Z materials as a function of photon energy.

agreement in the energy region ($100 \text{ keV} \leq E \leq 20 \text{ MeV}$), where the Compton interaction dominates. The effective atomic numbers are constant in the intermediate-energy region, whereas noticeable variation is observed for low- ($<20 \text{ keV}$) as well as high-energy regions. The effective atomic numbers calculated by the direct method are higher in photoelectric absorption and pair production compared with

the interpolation method. The effective atomic numbers calculated by XMuDat method are 5.53, 5.74, 5.67, 6.56, 6.33, and 6.21 for PE, PS, PP, PX, PC, and PA-6, respectively. The effective atomic numbers calculated by Auto- Z_{eff} for PP were found to be less than the direct and the interpolation methods. The independency of the effective atomic numbers on photon energy in intermediate-energy region observed

FIGURE 2: Comparison of the calculated effective atomic numbers of low-Z materials with human body tissues: (a) muscle (skeleton), (b) cortical bone, (c) thyroid, (d) adipose tissue and yellow bone marrow, and (e) spongiosa (skeleton).

in our investigation is similar to other various literatures for low- and high- Z elemental composites; however photoelectric absorption and pair production region need further experimental explanation [5]. Also large differences are observed in photoelectric absorption region, which is due to dependency on atomic number of the elements and photon energy. In Compton scattering region, it is found that the effective atomic numbers calculated by all three methods were the same order. The uncertainties in the effective atomic numbers computed by Auto- Z_{eff} method are of order of 1-2% for high photon energies.

Comparison of the theoretical effective atomic numbers with experimental data in the literature for PE, PS, and PP is given in Table 2(a). Also comparison of the theoretical effective atomic numbers with experimental data in the literature for PX, PC, and PA-6 is given in Table 2(b). From the tables, it has been clearly seen that the experimental values of the effective atomic numbers were consistent with the theoretical values.

4. Tissue Substitute and Human Body Tissues

The calculated $Z_{\text{eff,PI}}$ values of the low- Z materials were compared with the human body tissues in energy range 10 keV to 20 MeV as shown in Figures 2(a), 2(b), 2(c), 2(d), and 2(e). Various types of tissue substitutes for human organs and tissues are muscle (skeleton), cortical bone, thyroid, adipose tissue, yellow bone marrow, and spongiosa (skeleton). The calculated $Z_{\text{eff,PI}}$ values of the low- Z materials are found to be in very good agreement with the human body tissues with insignificant difference in the Compton scattering region. The following results were determined.

- (a) PE, PS, PX, and PA-6 were found equivalent to adipose and muscle (skeleton). The $Z_{\text{eff,PI}}$ values vary in the ranges of 3.45–7.89, 3.10–6.57, 2.67–5.30, 3.00–5.45, 3.61–6.63, and 3.27–6.19 for muscle (skeleton), adipose, PE, PS, PX, and PA-6, respectively.
- (b) Plaster of Paris (POP) was found equivalent to cortical bone whose $Z_{\text{eff,PI}}$ values vary in range 7.42–16.43 for POP and 6.02–16.17 for cortical bone respectively.
- (c) TH/L2 was found equivalent to thyroid tissue where the $Z_{\text{eff,PI}}$ values vary in range 3.47–7.34 for TH/L2 and 3.42–7.66 for thyroid respectively.
- (d) PP was found to be equivalent to yellow bone marrow and adipose tissues. The $Z_{\text{eff,PI}}$ values vary in the ranges of 2.67–5.30, 3.05–6.42, and 3.10–6.57 for polypropylene, yellow bone marrow, and adipose tissues, respectively.
- (e) PC was found equivalent to spongiosa (skeleton) and $Z_{\text{eff,PI}}$ values vary in the ranges of 3.71–6.16 for polycarbonate and 3.72–12.59 for spongiosa. The reason for large atomic numbers compared with PC in low-energy is due to high- Z elements (Na, Mg, P, S, and Ca) in spongiosa (photoelectric cross-section is dependent on Z^{4-5}).

5. Conclusions

In the present work, the theoretical methods were used to determine the effective atomic numbers of some low- Z materials (i.e., PE, PS, PP, PX, PA-6, POP, and TH/L2). The direct, the interpolation, and Auto- Z_{eff} methods demonstrate a good agreement in the effective atomic numbers in Compton scattering and pair production energy regions. A large difference in the effective atomic numbers calculated by the direct and the interpolation methods was observed in photoelectric and pair production regions. It was determined that PE, PS, PX, and PA-6 were equivalent to adipose and muscle (skeleton); POP was equivalent to cortical bone; TH/L2 was equivalent to thyroid tissue; PP was equivalent to yellow bone marrow and adipose tissues; PC was equivalent to spongiosa (skeleton).

Conflict of Interests

The authors declare that there is no conflict of interests regarding the publication of this paper.

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