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Assessment of methods for estimation of effective atomic numbers of common human organ and tissue substitutes: waxes, plastics and polymers

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Abstract – We calculated mass attenuation coefficients, effective atomic numbers and Kerma relative to air for human organ and tissue substitutes (*i.e.* wax, plastic and polymer materials). The effective atomic numbers of the tissue substitutes were calculated by the direct method, interpolation method, Auto-Z_{eff} software and single value XMuDat program and then compared. The calculated effective atomic numbers were also compared with available experimental data and a good agreement was observed. A large difference in effective atomic numbers calculated by the direct and interpolation methods was observed in photoelectric and pair-production regions. The direct method was found to be appropriate for effective atomic number computation in low-(>10 keV) and medium-($0.1 \leq E \leq 10$ MeV) photon energy regions. Kerma relative to air of the selected tissue substitutes was found to be dependent upon the atomic number and element compositions, which show a sharp peak due to K-edge absorption.

Keywords: wax / plastic / polymer / effective atomic number / Compton scattering / Kerma

1 Introduction

Simulation of radiation dose distribution in human organs and tissues is done by tissue-equivalent materials. The tissue-equivalent materials are used as tissue substitutes for various organs of the human body, having similar properties with respect to ionizing radiation interactions. Tissue substitutes are made of low-atomic-number materials (H, C, N, O, F, Cl, etc.). ICRU report 44 describes various types of tissue substitutes for human organs and tissues (ICRU, 1989) for diagnostic and therapeutic radiology, research, nuclear engineering, nuclear physics, health physics, radiation physics, medical physics, radiation dosimetry and radiation protection. Waxes, plastics and polymers are the choice for human organ and tissue substitutes due to their physical and chemical properties, ease of processing, significantly lower cost, low maintenance, and stability in the environment, which are used as a matrix of metals, and easy to shape. The waxes, plastics and polymers are used in phantom tissue substitutes for dosimetry services and calibration of radiation detectors.

Some photon interaction studies have been reported for low-Z materials in the low-energy photon region (Parthsaradhi *et al.*, 1992; Tejbir *et al.*, 2009, 2010; Murat and Yuksel, 2011). The effective atomic number of rubbers containing varying degrees of carbon contents has been investigated, showing a

range of effective atomic numbers (Elias *et al.*, 1983). Mass attenuation coefficients of tissue-equivalent materials used for human tissue simulation have been investigated, comparing densities and attenuation coefficients (Ferreira *et al.*, 2010). No detailed comparative study of photon interaction with the waxes, plastics and polymers used for tissue substitutes, shielding, dosimetry and medical physics is found in the literature at present. Keeping in mind the wide applications of the waxes, plastics and polymers, we investigated mass attenuation coefficients, μ_m, effective atomic numbers and Kerma relative to air, K_a, of the human organ and tissue substitutes given in Table 1.

Several authors have reported the effective atomic numbers for gaseous mixtures (Singh and Badiger, 2012), alcohols (Singh and Badiger, 2013), composite materials (Prasanna *et al.*, 2010), solutions (Kulwant *et al.*, 2001), dosimetric materials (Kiran and Venkata, 1997) and biological materials (Koç and Özyol, 2000; Shivalinge *et al.*, 2005; Manjunathguru and Umesh, 2006; Demir *et al.*, 2012). This study will be helpful for additional information and deciding the appropriate method for computation of the effective atomic numbers analogous to the experimental values.

2 Computational work

The mass attenuation coefficients and effective atomic numbers of the selected human organ and tissue substitutes

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Table 1. Elemental weight (%) of waxes, plastics and polymers for tissue substitution.

Serial Number	Tissue Substitutes	Element weight (%)						
		H	C	N	O	F	S	Cl
1	Poly-Vinyl-Chloride (PVC)	4.84	38.44	–	–	–	–	56.73
2	Synthetic Rubber (SR)	5.69	54.26	–	–	–	–	40.04
3	Epoxy-Resin (ER)	6.41	64.20	–	20.36	–	–	9.02
4	Poly-Chloro-Styrene (PCS)	6.19	69.63	–	–	–	–	24.18
5	Poly-PhenyleneSulfide (PPS)	3.73	66.63	–	–	–	29.65	–
6	Poly-Sulfone (PSU)	5.01	73.28	–	14.46	–	7.25	–
7	Poly-Ether-Sulfone(PES)	2.72	48.63	–	16.19	–	32.46	–
8	Modeling Clay (MC)	–	19.76	–	75.83	–	3.55	–
9	Natural Rubber (NR)	11.84	88.16	–	–	–	–	–
10	Poly-Propylene (PP)	14.37	85.63	–	–	–	–	–
11	Plastic-Scintillattor (PSc)	8.53	91.47	–	–	–	–	–
12	Bakelite (BK)	5.74	77.46	–	16.80	–	–	–
13	Teflon (TF)	–	24.02	–	–	75.98	–	–
14	Orange Articulation Wax (OAW)	2.72	82.00	7.37	7.82	–	0.08	–
15	Bee Wax (BW)	1.87	75.25	8.42	14.27	–	0.19	–

are derived by computation of mass attenuation coefficients and atomic cross-sections of the elements of the waxes, plastics and polymers. We computed the effective atomic numbers of the human organ and tissue substitutes by the direct method, interpolation method, Auto-Z_{eff} software and single value XMuDat program.

2.1 Mass attenuation coefficients

The μ_m ($=\mu/\rho$) values of human organ and tissue substitutes were calculated by the mixture rule, $(\mu/\rho)_{composite} = \sum_i^n w_i(\mu/\rho)_i$ where w_i is the proportion by weight and $(\mu/\rho)_i$ is the mass attenuation coefficient of the ith element, using the XCOM program (Berger *et al.*, 2010). Mass attenuation coefficients and attenuation cross-section data are available for 100 elements in the wide energy range from 1 keV to 100 GeV, which has been transformed into the user-friendly software package WinXCom (Gerward *et al.*, 2004) for the Windows platform. Using WinXCom software, mass attenuation coefficients and attenuation cross-section data are generated for the elements in the photon energy region from 1 keV to 20 MeV. The atomic number and atomic mass of the elements were taken from atomic weight of elements 2011, IUPAC (Michael *et al.*, 2013).

2.2 Effective atomic numbers

The effective atomic numbers of the composite material or compound can be calculated by the Auto-Z_{eff} software, direct method, interpolation method and single value XMuDat program. These methods use the elemental compositions and molar composition of the element in the compound materials.

2.2.1 Auto-Z_{eff}

Auto-Z_{eff} is user-friendly computer software in Visual Basic for rapid computation of the energy-dependent effective atomic number, average atomic numbers and spectral-weighted mean atomic numbers. Auto-Z_{eff} surpasses the dubious power-law approach. In this method, $Z_{eff,Auto}$ is determined via exploitation of the smooth correlation between the atomic cross-section and atomic number. A matrix of cross-sections was constructed spanning atomic numbers $Z = 1$–100 for photon energies ranging between 10 keV and 1 GeV, and cross-sections of poly-elemental media were calculated by linear additivity. The cross-section values are constructed with the cross-section matrix as a function of Z, and an effective Z number for each energy is obtained by interpolation (b-spline) of Z values between adjacent cross-section data (Taylor *et al.*, 2012).

2.2.2 Direct method

Computation of the effective atomic number, $Z_{eff,PI}$, of the waxes, plastics and polymers for total gamma photon interaction was carried out by the practical formula (Manohara *et al.*, 2008). The mass attenuation coefficients of the elements were obtained from the WinXCom computer program. The effective atomic number, $Z_{eff,PI}$, is given by

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

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

2.2.3 Interpolation method

The μ_m of the human organ and tissue substitutes are derived as mentioned above; the attenuation cross-section (σ) values of human organ and tissue substitutes are computed by using the relation:

$$\sigma = \frac{(\mu_m)}{N \sum_i \left(\frac{w_i}{A_i}\right)} \left(\frac{barns}{molecule}\right) \quad (2)$$

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

The attenuation cross-section values were interpolated in the attenuation cross-section values of the elements generated from WinXCom at selected energies to compute the effective atomic numbers using the logarithmic interpolation formula:

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

where σ_1 and σ_2 are the elemental cross-section (barn/atom) in between which the atomic cross-section σ of the waxes, plastics and polymers lies, and Z_1 and Z_2 are the atomic numbers of the elements (dimensionless) corresponding to the cross-sections σ_1 and σ_2, respectively.

2.2.4 XMuDat

The XMuDat computer program is able to produce a single-valued effective atomic number for compounds as well as mixtures (Nowotny, 1998). XMuDat uses the following formula for calculation of the effective atomic number:

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

where α_i is the fractional number of the electrons of the ith element, and m is a constant between 3 and 5. It is preferred that m is set to 3.6 for materials with $Z_{eff} < 6$, and 4.1 for materials with $Z_{eff} > 6$ (Jackson and Hawkers, 1981).

2.3 Kerma

Kerma relative to air of the human organ and tissue substitutes is derived by

$$K_a = \frac{K_{tissue\ substitutes}}{K_{Air}} = \frac{\left(\frac{\mu_{en}}{\rho}\right)_{tissue\ substitutes}}{\left(\frac{\mu_{en}}{\rho}\right)_{Air}} \quad (5)$$

Where $(\mu_{en}/\rho)_i$ of tissue substitutes and air is calculated from the compilation of Hubbell (1982).
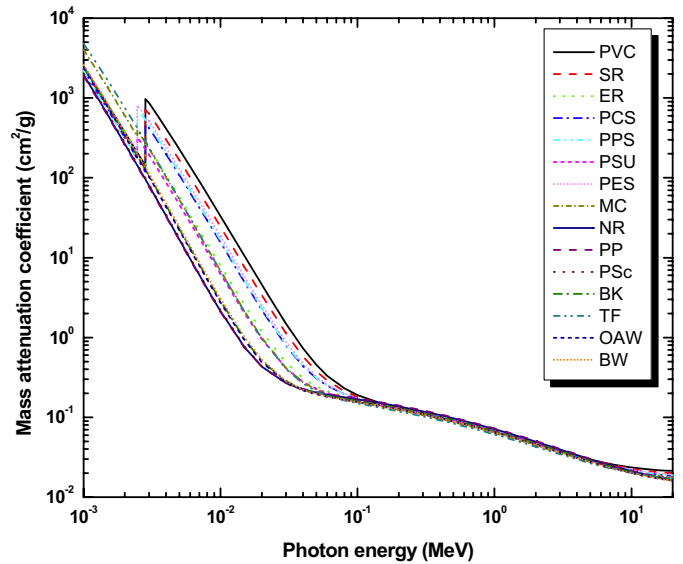

Fig. 1. Variation of mass attenuation coefficients with photon energy for waxes, plastics and polymers.

3 Results and discussion

The μ_m values of the waxes, plastics and polymers for the photon energies 10^{-3} to 20 MeV are shown in Figure 1 and explained by partial photon interactions (*i.e.* photoelectric absorption, Compton scattering and pair production). The effective atomic numbers computed by various methods in the photon energy region 0.01 to 20 MeV are given in Table 2. The calculated effective atomic numbers at different energies were compared with the experimental values and are shown graphically in Figure 2. The K_a is shown in Figure 3 and explained for photon energy, elemental atomic numbers and their composition dependencies.

3.1 Mass attenuation coefficient

The variation of the mass attenuation coefficient, μ_m, values of the tissue substitute materials with photon energy is shown in Figure 1. The μ_m values were found to be higher in low- as well as high-energy regions due to partial photon interaction processes, photoelectric absorption, Compton scattering and pair production in nuclear and electronic fields. It was observed that μ_m values were maximum at 1 keV, which decreased very fast with an increase in photon energy up to 50 keV for all the human organ and tissue substitutes except which contains $_{17}Cl$ and $_{16}S$ elements such as PVC, SR, ER, PCS, PPS, PSU, PES and MC. These elements have a sudden jump in μ_m values at 3 keV due to K-edge absorption. We found that a small amount of $_{32}S$ elements in the human organ and tissue substitutes did not appreciably alter μ_m values (in the case of BW). As photon energy increases, the μ_m values slowly decrease for all the human organ and tissue substitutes up to 10 MeV and then they gradually increase beyond 12 MeV photon energy. The μ_m values of PVC were found to be highest among all the selected human organ and tissue substitutes due to the maximum percentage composition of $_{17}Cl$

Table 2. Effective atomic numbers of tissue substitutes calculated by the Auto-Z_{eff}, direct and interpolation methods.

| Tissue substitutes	Method	Energy (MeV)				
		0.01	0.1	1	10	20
PVC	$Z_{eff,Auto}$	10.91	6.45	5.34	6.21	6.74
	$Z_{eff,PI}$	16.05	6.13	5.34	6.4	7.4
	Z_{eq}	10.93	6.48	5.37	6.23	6.77
SR	$Z_{eff,Auto}$	9.69	5.31	4.61	5.25	5.68
	$Z_{eff,PI}$	15.29	5.13	4.6	5.37	6.12
	Z_{eq}	9.73	5.34	4.63	5.27	5.7
ER	$Z_{eff,Auto}$	7.14	4.19	4.18	4.32	4.55
	$Z_{eff,PI}$	10.8	4.14	4	4.37	4.76
	Z_{eq}	7.15	4.21	4	4.35	4.59
PCS	$Z_{eff,Auto}$	8.46	4.57	4.17	4.61	4.94
	$Z_{eff,PI}$	13.94	4.47	4.16	4.69	5.23
	Z_{eq}	8.52	4.6	4.18	4.64	4.95
PPS	$Z_{eff,Auto}$	9.07	5.59	5.09	5.57	5.89
	$Z_{eff,PI}$	13.64	5.45	5.1	5.67	6.22
	Z_{eq}	9.08	5.61	5.1	5.6	5.9
PSU	$Z_{eff,Auto}$	6.88	4.45	4.3	4.57	4.77
	$Z_{eff,PI}$	9.71	4.4	4.3	4.62	4.95
	Z_{eq}	6.91	4.47	4.32	4.6	4.8
PES	$Z_{eff,Auto}$	9.63	6.45	5.85	6.37	6.69
	$Z_{eff,PI}$	13.73	6.26	5.85	6.49	7.07
	Z_{eq}	9.68	6.47	5.87	6.39	6.71
MC	$Z_{eff,Auto}$	8.14	7.7	7.63	7.67	7.69
	$Z_{eff,PI}$	8.96	7.68	7.62	7.68	7.73
	Z_{eq}	8.17	7.71	7.64	7.68	7.71
NR	$Z_{eff,Auto}$	4.69	2.96	2.92	3.11	3.27
	$Z_{eff,PI}$	5.42	2.95	2.92	3.14	3.38
	Z_{eq}	4.77	2.97	2.94	3.13	3.31
PP	$Z_{eff,Auto}$	4.21	2.27	2.25	2.4	2.55
	$Z_{eff,PI}$	5.3	2.69	2.67	2.87	3.1
	Z_{eq}	4.61	2.73	2.71	2.87	3.02
PSc	$Z_{eff,Auto}$	5.01	3.41	3.37	3.56	3.72
	$Z_{eff,PI}$	5.58	3.39	3.37	3.59	3.83
	Z_{eq}	5.01	3.44	3.4	3.6	3.75
BK	$Z_{eff,Auto}$	5.54	4.06	4	4.21	4.37
	$Z_{eff,PI}$	6.31	4.03	4	4.25	4.51
	Z_{eq}	5.63	4.06	4	4.23	4.4
TF	$Z_{eff,Auto}$	8.3	8.05	8	8.05	8.07
	$Z_{eff,PI}$	8.64	8.03	8	8.06	8.11
	Z_{eq}	8.36	8.06	8.01	8.06	8.08
OAW	$Z_{eff,Auto}$	5.84	4.91	4.86	5.02	5.13
	$Z_{eff,PI}$	6.3	4.89	4.87	5.05	5.23
	Z_{eq}	5.88	4.92	4.88	5.02	5.14
BW	$Z_{eff,Auto}$	6.13	5.34	5.29	5.42	5.51
	$Z_{eff,PI}$	6.61	5.32	5.29	5.45	5.6
	Z_{eq}	6.17	5.36	5.31	5.45	5.54
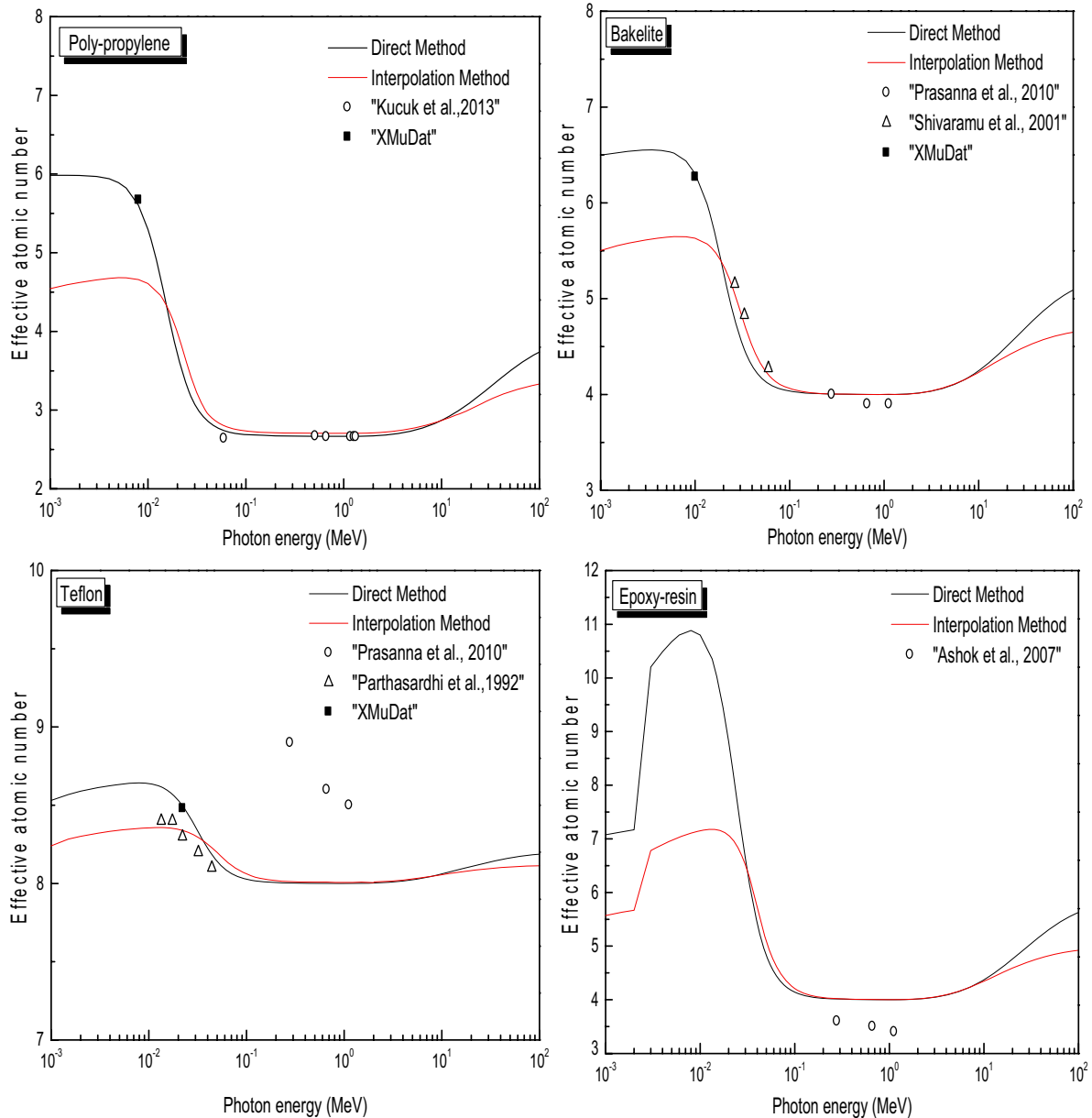
Fig. 2. Comparison of the calculated effective atomic numbers with the experimental values for waxes, plastics and polymers.

elements. It is to be noted that the μ_m values of TF, ER, PES and BW are higher than PVC below 3 keV.

The tissue substitutes (*i.e.* waxes, plastics and polymers) had elemental atomic numbers ranging from $1 < Z < 17$ (H: 1, C: 6, N: 7, O: 8, S: 16 and Cl: 17). The sharp decrease in μ_m values below 50 keV is due to the dominance of the photo absorption, where the photon interaction cross-section depends on Z^{4-5} and photon energy as $E^{-7/2}$. It is observed that the μ_m values were in the range of 10^3 to 10^4 cm^2/g (highest value) at photon energy 1–2 keV. As photon energy increases, the atomic number of the element plays a vital role: therefore, the μ_m values of PVC and SR were found to be the highest as they contain $_{17}$Cl contents of 56.73% and 40%, respectively. Beyond 50 keV, the Compton scattering process replaces photo absorption, where the photon interaction cross-section varies

linearly with Z and E^{-1}; thus, the μ_m values become almost independent of photon energy and decrease slowly up to 10 MeV. With a further increase in photon energy, the pair-production process dominates, where the interaction cross-section depends on Z^2 and logE, and hence the μ_m values begin to increase slowly.

3.2 Effective atomic numbers

The effective atomic numbers calculated by the different methods in the photon energy region 10 keV to 20 MeV for the human organ and tissue substitutes are given in Table 2. The effective atomic numbers below 10 keV were not compared due to high uncertainty ±25% by Auto-Z$_{eff}$ (Taylor *et al.*, 2012).

It was found that the effective atomic numbers computed by the Auto-Z_{eff}, direct and interpolation methods were in good agreement in the energy region of 50 keV to 10 MeV where the Compton interaction process dominates. The effective atomic numbers were found to be constant in the medium-energy photon region, whereas significant variation was observed in the lower-energy photon region (10–50 keV) as well as in the higher-energy photon region (10–20 MeV). The effective atomic numbers computed by the direct method are higher in the photo-absorption and pair-production regions compared with the interpolation method.

The variation in effective atomic numbers calculated by the Auto-Z_{eff} software, direct and interpolation methods for the human organ and tissue substitutes may be due to the basic concept and input parameters. In the Auto-Z_{eff} software, the effective atomic number is determined via exploitation of the smooth correlation between the atomic cross-section, atomic number and mass attenuation coefficients. The cross-sections of poly-elemental compounds are calculated by linear additivity. The effective atomic numbers of the human organ and tissue substitutes are calculated by interpolation (b-spline) of Z values of adjacent cross-section data of the cross-section matrix as a function of Z. The uncertainty in the effective atomic number by the Auto-Z_{eff} method is of the order of 1–2% at high photon energy.

3.3 Comparison with experiments

Comparison of the effective atomic numbers calculated using the direct and interpolation methods in the present work with the experimental values is shown in Figure 2. The experimental values of the effective atomic numbers of PP, BK and ER (Parthsaradhi *et al.*, 1992; Shivaramu *et al.*, 2001; Ashok *et al.*, 2007; Prasanna *et al.*, 2010; Kucuk *et al.*, 2013) in the Compton scattering-dominated region shows that the computed values in the present work are comparable. It is to be noted from the graphs that the effective atomic numbers in Compton region calculated by the direct and interpolation methods are in very good agreement. In the case of TF, the effective atomic number values are slightly distant from the calculation (Parthsaradhi *et al.*, 1992; Prasanna *et al.*, 2010). The reasons for this difference may be due to incoherent scattering cross-sections used for derivation of effective atomic numbers at the mentioned photon energies.

This comparative analysis shows that the effective atomic numbers derived by the direct method are appropriate in the photo-absorption region ($E > 10$ keV) and Compton-dominated region. Below 10 keV energy, experimental investigations are still required to find out the most suitable computational method for the effective atomic numbers. Our investigations into computation of effective atomic numbers signify that both the methods (direct and interpolation) used in our study are appropriate for Compton scattering for materials containing atomic numbers $1 < Z < 17$.

3.4 Kerma

The kerma relative to air, K_a variation of the tissue substitutes for photon energy (1 keV–20 MeV) is shown in Figure 3. K_a variation with photon energy represents variation of
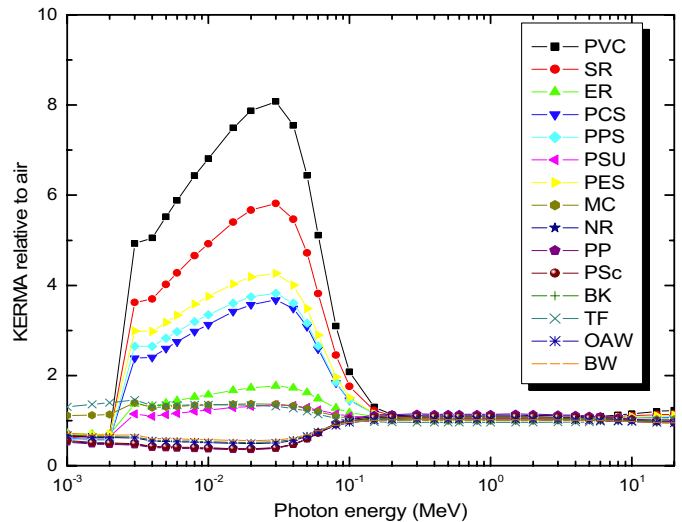

Fig. 3. Kerma relative to air as a function of photon energy for waxes, plastics and polymers.

the effective atomic numbers due to photo absorption, Compton scattering and pair production. It is to be noted that the K_a values of PVC, containing the highest-Z materials ($_{17}$Cl), reaches up to 8.08 at 3 keV compared with the others. Similarly SR, ER and PCS, containing $_{17}$Cl, and PPS, PSU, PES, BW, OAW and MC, containing $_{16}$S, show comparatively high K_a values. The peak value of K_a is due to the photoelectric effect around the K-absorption edge of $_{17}$Cl (2.82 keV) and $_{16}$S (2.47 keV) elements.

Figure 3 shows that the K_a value for PVC rises sharply from 0.57 to 4.93 and after this it builds up to 8.07 and then decreases slowly. The reason behind this may be that the K-edge absorption produces X-rays which are absorbed by valance electrons to eject from atomic bonding. These electrons with kinetic energy increase K_a values. As incident photon energy increases, the probability of K-edge absorption decreases; therefore, K_a values reach maximum values and then slowly decrease.

Below 100 keV photon energy, K_a values are found to be less than unity for those human organ and tissue substitutes which have a negligible or zero fraction of high-Z elements. We found that the K_a values of all the waxes, plastics and polymers are constant (~unity) above photon energy ~100 keV. It is also to be noted that K_a values are found to be <1 below 100 keV and >1 (1–1.1) above 100 keV for materials without K-edge absorption elements.

4 Conclusions

In the present study, we computed and compared the effective atomic numbers of the human organ and tissue substitutes by various methods (*i.e.* the direct method, interpolation method, Auto-Z_{eff} software and XMuDat program). The Auto-Z_{eff}, direct and interpolation methods are applicable at low photon energy (10 keV to 100 keV), where photo absorption dominates, and at medium photon energy (100 keV to 20 MeV), where Compton interaction dominates. A large

difference in effective atomic numbers by the direct and interpolation methods is observed in photoelectric and pair-production regions. The effective atomic numbers computed in the present work are in good agreement with the experiments. We also computed Kerma relative to air and found approximately unity except for chlorine-containing materials. Peaks in Kerma relative to air values are observed due to K-edge absorption of high-Z materials ($_{17}$Cl and $_{32}$S) in the photo-absorption region.

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