

Effective atomic numbers of some tissue substitutes by different methods: A comparative study

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ABSTRACT

Effective atomic numbers of some human organ tissue substitutes such as polyethylene terephthalate, red articulation wax, paraffin 1, paraffin 2, bolus, pitch, polyphenylene sulfide, polysulfone, polyvinylchloride, and modeling clay have been calculated by four different methods like Auto- Z_{eff} direct, interpolation, and power law. It was found that the effective atomic numbers computed by Auto- Z_{eff} direct and interpolation methods were in good agreement for intermediate energy region ($0.1 \text{ MeV} < E < 5 \text{ MeV}$) where the Compton interaction dominates. A large difference in effective atomic numbers by direct method and Auto- Z_{eff} was observed in photo-electric and pair-production regions. Effective atomic numbers computed by power law were found to be close to direct method in photo-electric absorption region. The Auto- Z_{eff} direct and interpolation methods were found to be in good agreement for computation of effective atomic numbers in intermediate energy region ($100 \text{ keV} < E < 10 \text{ MeV}$). The direct method was found to be appropriate method for computation of effective atomic numbers in photo-electric region ($10 \text{ keV} < E < 100 \text{ keV}$). The tissue equivalence of the tissue substitutes is possible to represent by any method for computation of effective atomic number mentioned in the present study. An accurate estimation of Rayleigh scattering is required to eliminate effect of molecular, chemical, or crystalline environment of the atom for estimation of gamma interaction parameters.

Key words: Atomic numbers, Compton scattering, gamma, mixture rule, tissue substitutes, Rayleigh scattering

Introduction

Simulation of depth-dose distribution inside human organs and tissues is made by tissue equivalent materials. The tissue equivalent materials are called as tissue substitutes for various tissues, organs of the human body, and tissue components having similar properties with respect to ionizing radiation. Average soft tissues are mainly composed of low-atomic number (Z) such as H, C, N, O, and so on.^[1] International Commission on Radiation Units (ICRU) report^[2] describes various types of tissue substitutes which are used in medicine, radiation

protection, and radiobiology to calibrate the radiation detectors and application in nuclear engineering for realistic body phantom.^[3,4] The effective atomic number is most vital parameters for tissue equivalence, radiation absorption, radiation scattering, and shielding effectiveness for gamma and neutron for compound materials.

Waxes are organic compounds which consist of long alkyl chains. Polymers are made from the monomer propylene which is rugged and highly resistant to the chemicals. Polymers are low- Z , nonflammable, light weight, high durability, ease processing, economical, and stable against environment. Nowadays, radiation shielding for gamma rays as well as neutron is made of polymer matrix lead shielding materials. Various types of waxes, plastics, and polymers are being used as tissue substitutes in field of medical, dosimetry, and radiological protection.

Investigators have studied effective atomic numbers of gaseous mixtures,^[5] composite materials,^[6] solutions,^[7] dosimetric materials,^[8,9] and biological materials.^[10-13] Several photon interaction studies are reported for low- Z materials^[14-17] for X- and gamma-ray photons. Rubbers containing varying degree of carbon show a wide range of effective atomic numbers.^[18] Mass attenuation coefficients of few common tissue substitutes have been reported.^[19] Recently, alcohol tissue substitutes for human organs have been investigated.^[20] The equivalence of tissue substitutes for experimental radiation

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physics has been reported by $(\mu/\rho)_{\text{substitute}}/(\mu/\rho)_{\text{tissue}}$ for energy 0.01-100 MeV and linear attenuation coefficients at 60-80 keV for radiation characteristic of tissue substitutes.^[21]

The bolus tissue substitute is easily made, inexpensive, and moldable during treatment.^[22,23] The paraffin is lipid equivalent material^[2] and polyethylene terephthalate is a good skeleton-cartilage substitute.^[2] Red articulation wax is used for dosimetry phantom preparation and pitch is very good skin equivalent material. The effective atomic number dependency upon photon energy is evaluated by various methods like Auto- Z_{eff} ,^[24] direct method,^[25] and logarithmic interpolation method. These methods use different input parameters (e.g. atomic cross-sections, atomic numbers, and attenuation coefficients) for computation of effective atomic numbers. The direct and interpolation methods use mixture rule^[26,27] for computation of mass attenuation coefficients of the compound or mixture. The mixture rule is simple additive law for weighted sum of mass attenuation of constituent elements. The photon interaction processes are energy dependent and photo-electric effect ($E < 0.1$ MeV) is largely energy dependent. Appreciable differences between experiment and theoretical mass attenuation coefficients of polymers (59.5 keV), vitamins (30.82-59.54 keV), amino acids (8.04-80.99 keV), Au alloys (59.5 keV), and brass alloys (81 keV) are noted.^[13,28-31] Effective atomic numbers of high-Z compounds like magnesium ferrite and borosilicate glass are observed to be following the mixture rule in low-energies.^[32,33] It is expected that the effective atomic numbers computed by different theoretical methods should be identical in magnitude for the compound materials at selected energies. Presently, such type of comparative study is not found in the literature and was studied first time.

In view of above, we have chosen some important tissue substitutes ($1 \leq Z < 18$) given in Table 1 for computation of effective atomic numbers by Auto- Z_{eff} , direct, interpolation, and power law methods for various medical applications. This study will benefit for readily available effective atomic numbers of the tissue substitutes and choice for appropriate method for computation of effective atomic numbers.

Computational work and theoretical background

Mass attenuation coefficients and effective atomic numbers of compound materials are derived by mixture rule using mass attenuation coefficients and atomic cross-sections of the elements. In our study, we have computed the mass attenuation coefficients and effective atomic numbers of the tissue substitutes given in Table 1. These materials have been taken from the references.^[2,34,35] The attenuation cross-section data can be found for 100 of elements in energy range of 1 keV-100 GeV by XCOM program.^[36] The XCOM data have been transformed to user-friendly software package WinXCom^[37] for the window platform which is easily exportable in the excel files. Using WinXCom, mass attenuation coefficients and attenuation cross-section data were generated for the elements in photon energy region 10 keV-20 MeV. The atomic numbers and atomic masses of the elements are taken from atomic weight of elements 2009, International union of Pure and Applied Chemistry.^[38]

Mass attenuation coefficients

The mass attenuation coefficient, μ/ρ value for the selected tissue substitutes was estimated by Bragg's law or mixture rule.^[26,27] The μ/ρ values of tissue substitutes were calculated by mixture rule $((\mu/\rho)_{\text{tissuesubstitute}} = \sum_i^n w_i (\mu/\rho)_i)$ where w_i is the proportion by weight and $(\mu/\rho)_i$ is mass attenuation coefficient of the i^{th} element. The quantity w_i is given by $w_i = n_i A_i / \sum_i^n n_i A_i$ 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 linear attenuation coefficients of the tissue substitutes can be calculated by multiplication of μ/ρ and density.

Auto- Z_{eff}

Auto- Z_{eff} is user-friendly software in visual basic for rapid computation of the energy-dependent effective atomic numbers, average atomic numbers, and spectral-weighted mean atomic numbers. Auto- Z_{eff} surpasses dubious power-law approach. In this method, $Z_{\text{eff}}^{\text{Auto}}$ is determined

Table 1: Elemental composition of tissues substitutes

Tissue substitutes	Weight percentage					
	H	C	N	O	S	Cl
Polyethylene terephthalate	4.20	62.50	0.00	33.30	0.00	0.00
Red articulation wax	0.36	80.17	11.23	8.14	0.09	0.00
Paraffin 1 (PF1)	0.61	81.73	0.74	16.81	0.10	0.00
Paraffin 2 (PF2)	0.68	79.61	9.63	9.94	0.14	0.00
Bolus (BL)	0.50	82.22	0.78	16.41	0.09	0.00
Pitch (PT)	0.19	42.18	0.42	56.76	0.46	0.00
Polyphenylene sulfide	3.73	66.63	0.00	0.00	29.65	0.00
Polysulfone	5.01	73.28	0.00	14.46	7.25	0.00
Poly-vinyl-chloride	4.84	38.44	0.00	0.00	0.00	56.73
Modeling clay	0.00	19.76	0.00	75.83	3.55	0.00

Cl: Chlorine

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 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 for any energy is obtained by interpolation of Z values between adjacent cross-section data.^[24]

Direct method

Computation of the effective atomic number, $Z_{\text{eff, PI}}$ of the selected tissue substitutes for total gamma photon interaction has been carried out by practical formula.^[25] The mass attenuation coefficients of the elements have been obtained from WinXcom computer program. The effective atomic number, $Z_{\text{eff, PI}}$ is given by

$$Z_{\text{eff, PI}} = \frac{\sum_i f_i A_i \left(\frac{\mu}{\rho}\right)_i}{\sum_i \frac{f_i A_i}{Z_i} \left(\frac{\mu}{\rho}\right)_i} \dots\dots(1)$$

where the ratio, A/Z , between the atomic mass and the atomic number is approximately constant. The effective atomic number for photon energy absorption (Z_{PEAeff}) can be obtained from Eq. (1) by substituting the mass energy absorption coefficient, μ_{en}/ρ , for mass attenuation coefficient.

Interpolation method

Mass attenuation coefficient values of the materials, μ_m , are derived by mixture rule as mentioned above. The attenuation cross-section (σ) values of tissue substitute materials are computed by using the relation:

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

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 tissue substitute material and A_i the atomic weight of the i^{th} element in a molecule. w_i and A_i are both dimensionless quantities.

The attenuation cross-section values obtained 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;

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

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

Power law method

The effective atomic number, $Z_{\text{eff, PL}}$, of a tissue substitute material by power law can be calculated according to the following equation:

$$Z_{\text{eff, PL}} = \sqrt[x]{a_1 Z_2^x + a_2 Z_2^x} + \dots\dots(4)$$

with

$$a_j = \frac{n_i(Z_i)}{\sum_i n_i(Z_i)}$$

where a_1, a_2, \dots are the fractional contents of electron belonging to element Z_1, Z_2, \dots , respectively, n_i is the number of electrons, in one mole, belonging to each element Z_i and N_A is the Avogadro’s number. The x values are in 2.94^[39] and 3.5^[40] ranges.

Errors

Auto- Z_{eff} software calculates effective atomic numbers with errors of 1%-2% for photon energies 10 keV-1000 MeV. This errors increase to 25%-50% below 10 keV.^[24] The errors in mass attenuation coefficients of the elements is about 1% for low- Z ($1 < Z < 8$) in the energy region where Compton scattering dominates (30 keV-100 MeV).^[41] Below 30 keV and above 100 MeV, the errors are as much as 5%-10%. For medium- Z elements sodium through copper, the errors are 1%-2% for energies 10 keV-1 MeV and 2%-3% for energies 1-100 MeV. Medical, biological, and industrial, applications and transportation tend to use sources with photon energies above 5 keV, so that the errors in our results may not have any practical impact. The power law method is an inaccurate method as the exponent of 2.94 relates to an empirical formula for the photoelectric process which incorporates a “constant” of 2.64×10^{-26} , which is in fact not a constant but rather a function of the photon energy. A linear relationship between $Z^{2.94}$ has been shown for a limited number of compounds for low-energy x-rays.^[42]

Result and Discussion

Variation of mass attenuation coefficients of selected tissue substitutes is shown in Figure 1 for photon energy range 1 keV-100 GeV. The effective atomic numbers of the selected tissue substitutes by Auto- Z_{eff} , direct, interpolation methods, and power law is shown in Figure 2a-j. The variations of these parameters were explained in detail in the next section.

Mass attenuation coefficient

Figure 1 shows the mass attenuation coefficient, μ/ρ variation of tissue substitutes in photon energy range 1 keV-100 GeV. The Figure 1 shows that the μ/ρ values of the tissues substitutes decrease with increase in the photon energies in low-energy, minimum in intermediate-energy, and constant in high-energy region. The variation in μ/ρ values with energy

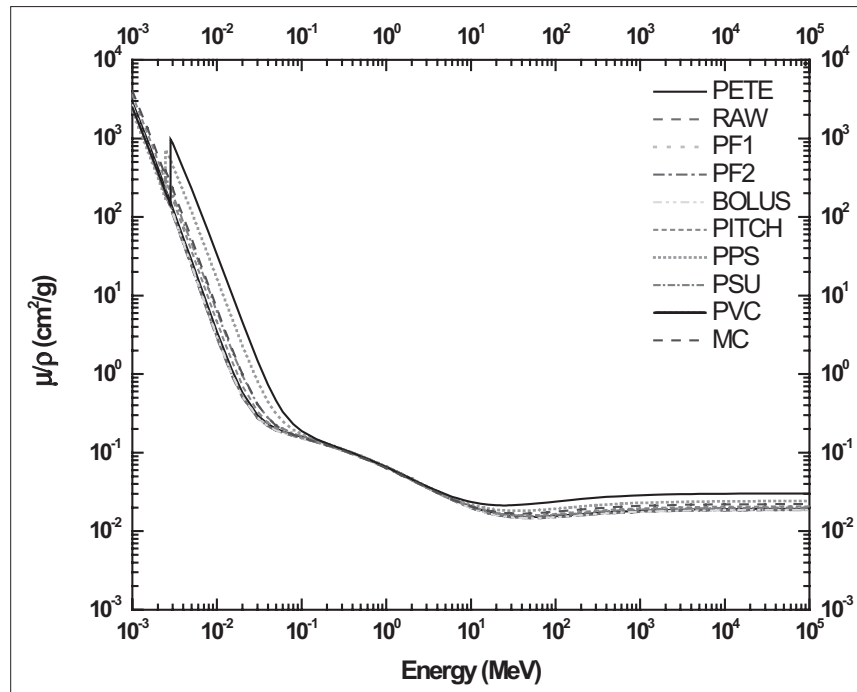


Figure 1: Mass attenuation coefficients of tissue substitutes in photon energy range 1 keV-100 GeV

can be explained by partial photon interaction processes as the dependence of the total atomic cross-section on atomic number and photon energy. The interaction cross-section is directly proportional to $Z^{-4.5}/E^{3.5}$ for photo-electric absorption in low-energy; therefore, μ/ρ values of the tissues substitutes reduces sharply. In Compton scattering region (intermediate-energy region), the interaction cross-section is dependent upon Z/E , whereas cross-section is directly proportional to Z^2 for pair-production (high-energy). The μ/ρ values of all the selected tissues substitutes merges in Compton scattering ($100 \text{ keV} < E < 10 \text{ MeV}$) region.

The μ/ρ values of Griffith breast tissue substitutes and breast of human body tissue [2] were compared with the selected tissue substitutes. It was found that the Polyethylene Terephthalate polyphenylene sulfide, and polysulfone, can replace Griffith tissue in photon energy region 0.10-10 MeV, whereas Polyethylene Terephthalate is most suitable for entire energy region

Effective atomic number

Effective atomic numbers of the selected tissue substitutes by different four methods (Auto- Z_{eff} , direct, interpolation, and power law) is shown Figure 2a-j. From Figure 2, it is observed that the effective atomic numbers computed by Auto- Z_{eff} , direct and interpolation methods are in good agreement and almost identical in the energy region 0.1-5 MeV where the Compton interaction dominates. The effective atomic number values were found constant in the intermedium photon energy region, whereas significant variation was observed in the lower (0.01-0.1 MeV) as well as in the higher-energy regions (5-20 MeV). The effective

atomic numbers computed by direct method were higher in photo-electric absorption and pair-production regions as compared with interpolation method. The effective atomic numbers calculated by Auto- Z_{eff} were 6.01-6.23, 4.55-6.07, 5.90-6.27, 5.84-6.21, 5.96-6.28, 6.87-7.22, 5.09-9.07, 4.30-6.88, 5.34-11.02, and 7.63-8.14 for RAW, PETE, PF1, PF2, BOLUS, PITCH, PPS, PSU, PVC and MC- respectively, by direct method were 6.01-6.46, 4.55-6.81, 5.90-6.6, 5.84-6.52, 5.96-6.58, 6.87-7.63, 5.11-13.64, 4.30-9.71, 5.34-16.05, and 7.62-8.96 for RAW, PETE, PF1, PF2, BOLUS, PITCH, PPS, PSU, PVC and MC, respectively; whereas by interpolation method 6.00-6.29, 4.57-6.09, 5.91-6.34, 5.85-6.27, 5.97-6.35, 6.88-7.28, 5.11-9.08, 4.40-6.91, 5.37-11.02, and 7.64-8.18 for RAW, PETE, PF1, PF2, BOLUS, PITCH, PPS, PSU, PVC, and MC, respectively. The effective atomic numbers by power law is shown in the graphs for x equals to 2.94 and 3.5. The independency of effective atomic numbers on photon energy in Compton dominant region can be found in various literatures for materials containing low- and high-Z elements; however, photo-electric absorption and pair-production region are not found experimentally.^[6,7,9] The effective atomic numbers computed by power law were found to be in the photo-electric absorption region close to direct method. In Compton scattering region, it was found that the effective atomic numbers by all the three methods were in good agreement.

The variation in effective atomic numbers of the tissue substitutes by Auto- Z_{eff} , direct, and interpolation methods may be due to basic concept and input parameters for computation. In the Auto- Z_{eff} effective atomic numbers

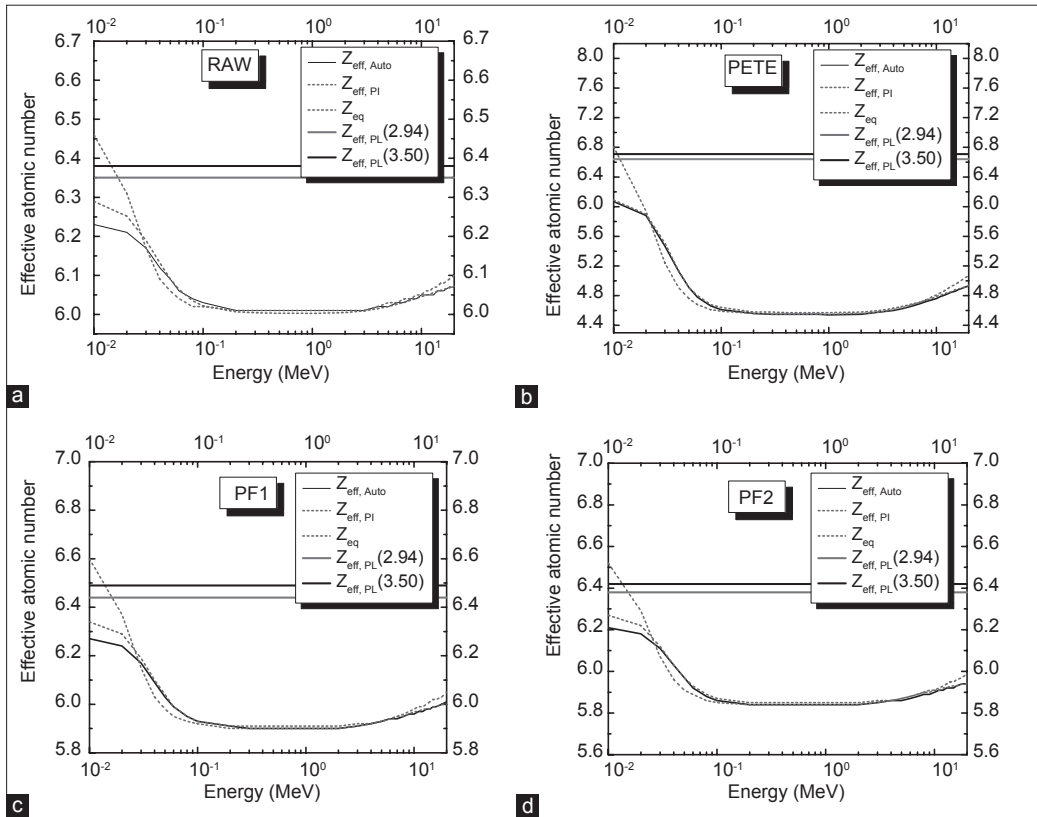


Figure 2a-d: Effective atomic numbers of Red Articulation Wax, Polyethylene Terephthalate, Paraffin 1, Paraffin 2, Bolus, Pitch, Poly-Phenylene Sulfide, Poly-Sulfone, Poly-vinyl-chloride and Modeling Clay for photon energy ranges from 10 keV to 20 MeV by Auto-Zeff, direct, interpolation, and power Law

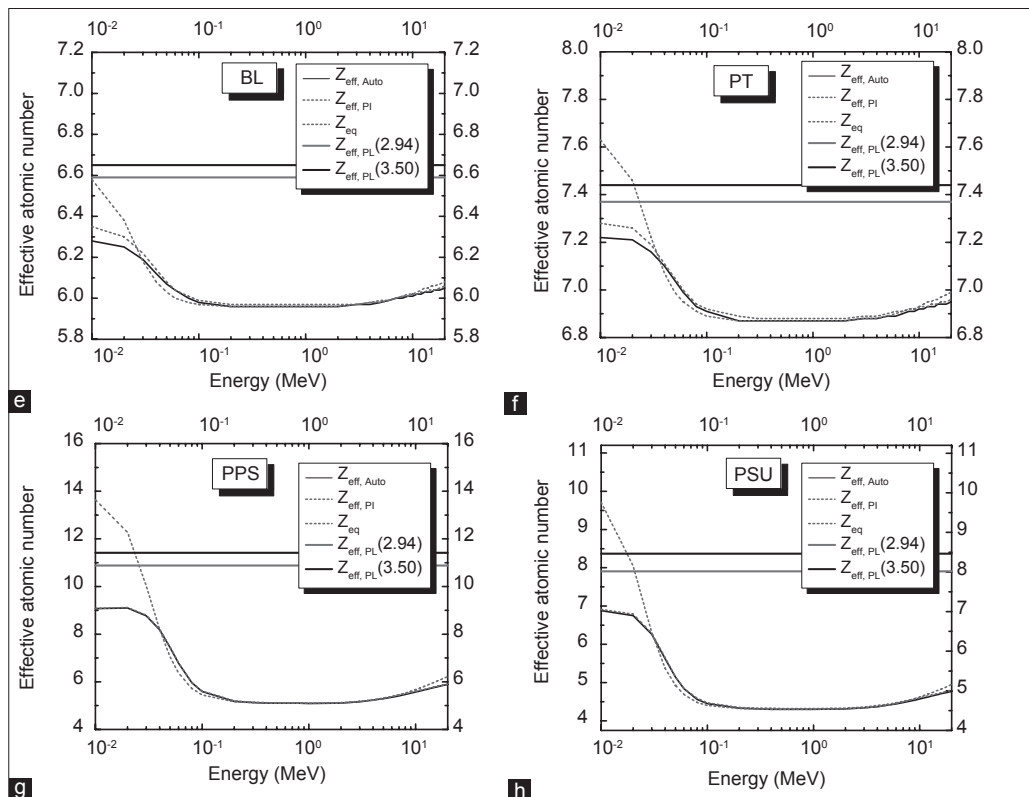


Figure 2e-h: Effective atomic numbers of Red Articulation Wax, Polyethylene Terephthalate, Paraffin 1, Paraffin 2, Bolus, Pitch, Poly-Phenylene Sulfide, Poly-Sulfone, Poly-vinyl-chloride and Modeling Clay for photon energy ranges from 10 keV to 20 MeV by Auto-Zeff, direct, interpolation, and power Law

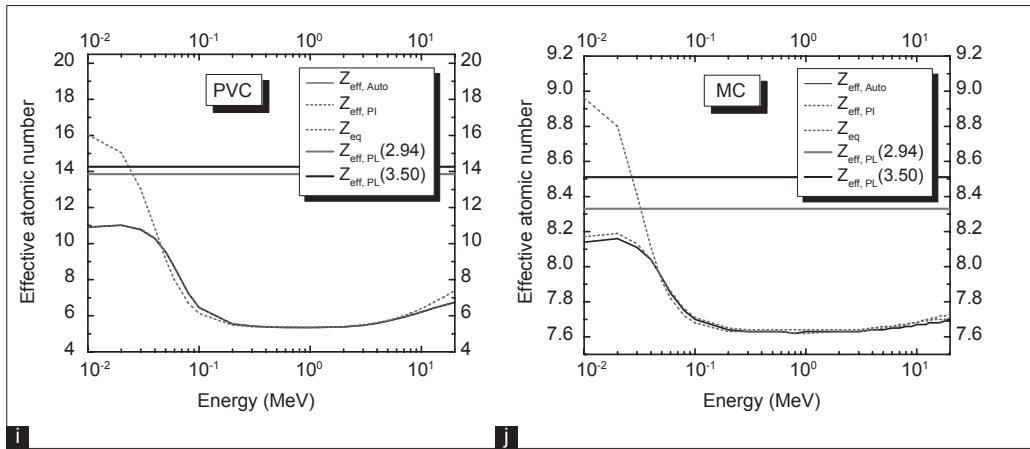


Figure 2i-j: Effective atomic numbers of Red Articulation Wax, Polyethylene Terephthalate, Paraffin 1, Paraffin 2, Bolus, Pitch, Poly-Phenylene Sulfide, Poly-Sulfone, Poly-vinyl-chloride and Modeling Clay for photon energy ranges from 10 keV to 20 MeV by Auto-Zeff, direct, interpolation, and power Law

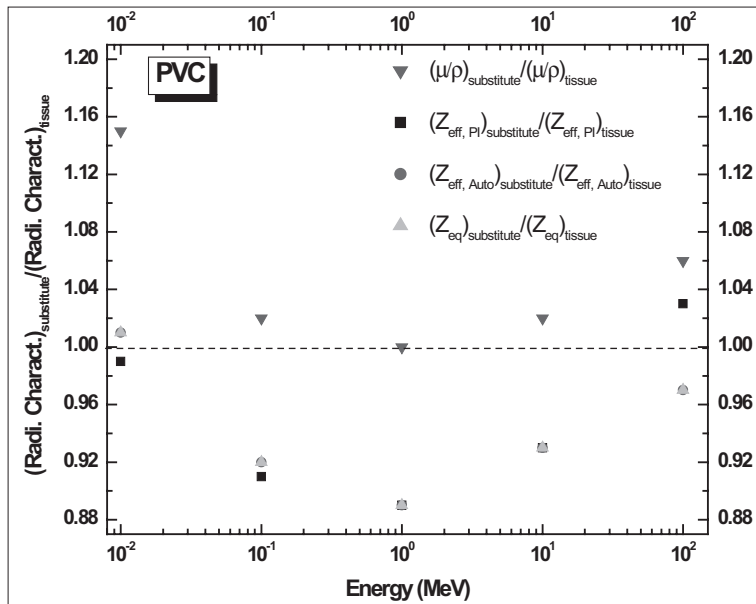


Figure 3: Comparison of radiation characteristics (mass attenuation coefficients and effective atomic number) of poly-vinyl-chloride and cortical bone at photon energies 0.01, 0.1, 1, 10, and 100 MeV

are determined via exploitation of the smooth correlation between atomic cross-sections, atomic numbers, and mass attenuation coefficients. The cross-sections of polyelement compounds are calculated by linear additivity. The effective atomic numbers of the tissue substitutes was calculated by interpolation of Z of adjacent cross-section data of cross-section matrix as function of Z. Large variation in effective atomic number by direct method and interpolation method is observed because of different weight fractions are given as input in computation.

For tissue equivalence of the tissue substitutes, a graph for substitute (PVC) and tissue (cortical bone) has been plotted in Figure 3. The ratio of effective atomic numbers by direct, Auto-Z_{eff}, and interpolation for substitute to tissue along with $(\mu/\rho)_{substitute} / (\mu/\rho)_{tissue}$ reported by White for

photon energies 0.01, 0.1, 1, 10, and 100 MeV^[21] are shown on abscissa; whereas radiation characteristics (effective atomic numbers and mass attenuation coefficients) are shown in the ordinate. It is evident from the Figure 3 that the tissue equivalence of PVC is far away for $(\mu/\rho)_{substitute} / (\mu/\rho)_{tissue}$ method in low energy (<0.1 MeV) compared with effective atomic number method. In Compton scattering region, a good correlation is to be noted. With increase in the photon energy (>10 MeV), the deviations by both the methods were observed of same order. The ratio of Z_{eff, PL} of PVC to cortical bone was found to be 1.05 and 1.03 for x values of 2.94 and 3.5 respectively. Therefore, the double-valued Z_{eff, PL} using power law method shows insignificant variation of the radiation characteristics of PVC and cortical bone. The difference between the ratios of effective atomic numbers of tissue substitutes to tissues

using above methods (direct, Auto- Z_{eff} , and interpolation) was noted insignificant. Therefore, it can be concluded that the tissue equivalence of the tissue substitutes is possible to represent by using above methods (Auto- Z_{eff} , direct, interpolation) for computation of effective atomic numbers.

In case of photo-electric absorption region, the interaction process is affected near absorption edges of the elements which may perturb the wave-function of the compound or mixture. The results support the conclusion elaborated in earlier several reports^[41-42] that the mixture rule is valid for the evaluation of photon attenuation coefficients for compounds in Compton scattering region. Therefore, mixture rule is limited to Compton scattering region and demand for further experimental data for smoothening of the interaction cross sections and its applicability in photo-electric ($10 \text{ keV} < E < 100 \text{ keV}$) and pair-production regions ($E > 10 \text{ MeV}$). From Figure 2, it is evident that in photo-electric absorption region the effective atomic numbers by interpolation method and Auto- Z_{eff} are far away from direct method. The experimental data for effective atomic numbers of various compounds/mixtures^[13,28-31] and power law method results were found to be closest to the direct method; therefore, it is concluded that the direct method may be appropriate for computation of effective atomic numbers in photo-electric absorption region.

Discrepancies

The mass attenuation coefficients of chemical compound or mixture is evaluated by weighted sum of mass attenuation coefficients of the constituent elements using mixture rule. The mixture rule is not valid near k-absorption edge of the compounds and mixtures.^[43-46] The mixture rule does not consider the molecular, chemical, or crystalline environment of the atom which results in change in the atomic wave-function. With the exception of the fine structure region above absorption edge ($>10 \text{ keV}$) errors from these sources are expected to be a few percent, whereas at low energies ($10\text{-}100 \text{ eV}$), errors of as much as a factor of two can occur. In case of Auto- Z_{eff} , the cross-sections of poly-elemental media are also calculated by linear additive method.

The study upon molecular, chemical, or crystalline environment of the atom^[43-44] reveals that there is requirement for revision of the cross-section and attenuation coefficients libraries in photo-electric absorption region. The reason behind is that the actual energy at which a particular photo-electric absorption edge of an element occurs is dependent on the chemical state of the absorbing atom and the nature of the chemical environment: For example, a chemical shift in the position of the k-edge in iron can be seen as the oxidation state of the atom is changed.^[47] High-resolution studies show that within the edge region the structure depends on the electronic structure of the absorbing atom. The actual height of the edge is also

sensitive to the atomic environment and hence there may be uncertainty in determining the k-jump ratios.^[48] The errors in theoretical estimates of Rayleigh scattering may be the cause of part of the deviation in absorption coefficient as observed.^[48] It may be concluded that the theoretical estimates for Rayleigh scattering for the photon energies very close to the K-edge are not accurate. An accurate estimation of Rayleigh scattering is required to eliminate effect of molecular, chemical, or crystalline environment of the atom. Therefore, the discrepancies in the effective atomic number may be diminished by considering the molecular, chemical, or crystalline environment of the atom for deriving the atomic cross-section, interaction and attenuation coefficients.

Conclusions

In the present study, we have compared effective atomic numbers of some important tissue substitutes by four methods (i.e., Auto- Z_{eff} , direct method, interpolation method, and power law). The direct and power law methods are applicable in low-photon energy ($10 \text{ keV} < E < 100 \text{ keV}$) where photo-absorption dominates and intermediate-energy ($0.1 \text{ MeV} < E < 10 \text{ MeV}$) where Compton scattering interaction dominates. A large difference in effective atomic numbers by direct method and Auto- Z_{eff} methods was observed in photo-electric and pair-production regions. An accurate estimation of Rayleigh scattering is required to eliminate effect of molecular, chemical, or crystalline environment of the atom. Therefore, the discrepancies in the effective atomic number may be diminished by considering the molecular, chemical, or crystalline environment of the atom for deriving the atomic cross-section, interaction, and attenuation coefficients. Direct method was found to be an appropriate method for deriving effective atomic numbers in photo-electric region ($10 \text{ keV} < E < 100 \text{ keV}$).

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