

# Determining the mass attenuation coefficient, effective atomic number, and electron density of raw wood and binderless particleboards of *Rhizophora* spp. by using Monte Carlo simulation



Mohammad W. Marashdeh<sup>a,b,\*</sup>, Ibrahim F. Al-Hamarnah<sup>a,c</sup>, Eid M. Abdel Munem<sup>b</sup>, A.A. Tajuddin<sup>b</sup>, Alawiah Ariffin<sup>b</sup>, Saleh Al-Omari<sup>d</sup>

<sup>a</sup> Department of Physics, College of Sciences, Al Imam Mohammad Ibn Saud Islamic University (IMSIU), P.O. Box 90950, Riyadh 11623, Saudi Arabia

<sup>b</sup> School of Physics, Universiti Sains Malaysia, Minden, 11800 Penang, Malaysia

<sup>c</sup> Department of Physics, Faculty of Science, Al-Balqa Applied University, Salt 19117, Jordan

<sup>d</sup> Department of Physics, Faculty of Science, The Hashemite University, Zarqa 13115, Jordan

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## ABSTRACT

*Rhizophora* spp. wood has the potential to serve as a solid water or tissue equivalent phantom for photon and electron beam dosimetry. In this study, the effective atomic number ( $Z_{eff}$ ) and effective electron density ( $N_{eff}$ ) of raw wood and binderless *Rhizophora* spp. particleboards in four different particle sizes were determined in the 10–60 keV energy region. The mass attenuation coefficients used in the calculations were obtained using the Monte Carlo N-Particle (MCNP5) simulation code. The MCNP5 calculations of the attenuation parameters for the *Rhizophora* spp. samples were plotted graphically against photon energy and discussed in terms of their relative differences compared with those of water and breast tissue. Moreover, the validity of the MCNP5 code was examined by comparing the calculated attenuation parameters with the theoretical values obtained by the XCOM program based on the mixture rule. The results indicated that the MCNP5 process can be followed to determine the attenuation of gamma rays with several photon energies in other materials.

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## Introduction

Materials used as solid water and tissue equivalent phantoms have to exhibit radiological characteristics similar to those of water. Hence, the tissue-equivalence for photon beams can be ensured by checking the total mass attenuation coefficient ( $\mu_m$ ), effective atomic number ( $Z_{eff}$ ), and effective electron density ( $N_{eff}$ ) [1,2]. Numerous experimental and theoretical investigations have been conducted to determine the interaction parameters of X-rays and  $\gamma$ -rays with elements, compounds, and mixtures. These studies aimed to determine the values of  $\mu_m$  and  $Z_{eff}$  [3–5] to represent the attenuation of radiation in compounds and mixtures, as well as in dose calculations in radiation therapy [6]. The accurate values of radiation interaction parameters in several materials are invaluable in many applied fields of science, such as nuclear

and radiation physics, radiation protection and dosimetry, nuclear diagnostics and nuclear medicine, as well as agricultural, environmental, and industrial studies. Hubbell and Seltzer [7] tabulated the  $\mu_m$  in a wide energy range (1–20 MeV) for all elements ( $Z = 1$  to 92) and 48 additional substances of dosimetric interest. As an alternative technique, Berger and Hubbell [8] developed a computer program named XCOM for calculating the attenuation coefficients of elements, compounds, and mixtures in a wide range of photon energies. Gerward et al. [9] converted this program to the Windows platform and named it WinXcom. This program is based on the mixture rule for calculating the partial and total mass attenuation coefficients for all standard elements and mixtures and selected energies.

*Rhizophora* spp. is a type of mangrove wood that exhibits the characteristics of ionizing radiation interaction similar to those of water, as well as similarities in radiometric properties with other standard phantom materials in radiation dosimetry [10–13]. However, the natural wood of *Rhizophora* spp. suffers from a number of drawbacks, such as inhomogeneity of density and propensity to grow mold, and it becomes slimy, warped, and cracked with time, which limit its use as a tissue-equivalent phantom material. Hence,

\* Corresponding author at: Department of Physics, College of Sciences, Al Imam Mohammad Ibn Saud Islamic University (IMSIU), P.O. Box 90950, Riyadh 11623, Saudi Arabia.

E-mail addresses: [mwmarashdeh@gmail.com](mailto:mwmarashdeh@gmail.com), [mwmarashdeh@imamu.edu.sa](mailto:mwmarashdeh@imamu.edu.sa) (M.W. Marashdeh).

binderless *Rhizophora* spp. particleboard is preferable than raw wood because of its accessibility to be fabricated easily into homogenous slabs without cracks [11,14]. In the current study, the photon interaction for *Rhizophora* spp. wood is evaluated. The effective atomic number ( $Z_{eff}$ ) and effective electron density ( $N_{eff}$ ) of raw *Rhizophora* spp. wood and *Rhizophora* spp. binderless particleboard in four different particle sizes, as well as that of pure liquid water and young-age breast tissue, are calculated in the energy range from 10 keV to 60 keV. The mass attenuation coefficients used in these calculations are obtained using the Monte Carlo N-Particle (MCNP5) simulation code. The obtained data are compared with the theoretical values calculated using the XCOM program based on the mixture rule. The dependencies of these parameters among the investigated samples over the photon energy considered, as well as the relative differences, are examined and discussed accordingly.

The values of  $Z_{eff}$  and  $N_{eff}$  in the 10–60 keV energy region of *Rhizophora* spp. wood classified as a tissue equivalent material have not been reported. Banjade et al. [10] reported an estimated average value of 7.09 for  $Z_{eff}$  of *Rhizophora* spp. wood, but did not consider the variation over energy. Thus, we conducted this study as a sequel to the work conducted by Marashdeh et al. [12]. The present calculations are performed on the same composite materials of the previous study, but in a wider range of energy (10–60 keV). The present work is important because accurate values of attenuation parameters are necessary to establish the regions of validity of theory-based parameterization, in addition to providing essential data in such diverse fields as tomography, X-ray and  $\gamma$ -ray fluorescence studies, and radiation biophysics.

## Theory

The interaction of radiation with matter is important in radiation, nuclear, medical, biophysics, and other applied sciences. The probability of photon interaction by one physical process or another per unit distance traveled is called the linear attenuation coefficient or macroscopic cross section and is denoted by  $\mu_r$ . The mass attenuation coefficient  $\mu_m$  is a density independent coefficient, which is a measure of the degree of absorption or scattering of radiation by a chemical species or substance at a given wavelength per unit mass. The coefficient  $\mu_m$  (in  $\text{cm}^2 \text{g}^{-1}$ ) is obtained by dividing  $\mu_r$  by the density  $\rho$  of the absorber material. A collimated beam of radiation penetrating a material with mass-per-unit-area  $x$  is attenuated according to the exponential absorption law, Eq. (1) [15]:

$$\frac{I}{I_0} = e^{-(\mu_r/\rho)x} = e^{-\mu_m x} \quad (1)$$

where  $I_0$  and  $I$  are, respectively, the intensity of un-attenuated and attenuated radiation in the absorber medium. Then Eq. (1) can be rewritten as:

$$\ln \left( \frac{I_0}{I} \right) = \mu_m x \quad (2)$$

Eq. (2) is a linear equation for the mass-per-unit-area  $x$  of the target, and the mass attenuation coefficient  $\mu_m$  is thus directly obtained as the slope of this straight line. According to Nordfors criteria [16], the optimum range of attenuation coefficients should match to satisfy the condition ( $0.5 < \mu_m x < 5.0$ ).

Attenuation of X-rays and  $\gamma$ -rays in matter is related to density and atomic number. The effective atomic number ( $Z_{eff}$ ) of compounds and composite materials plays a crucial role in representing the attenuation of X-rays and  $\gamma$ -rays [5], particularly for dose calculations in radiation therapy [4]. This parameter has gained considerable interest in terms of radiation interaction with

composite materials.  $Z_{eff}$  can be calculated based on knowledge of the total atomic cross-section  $\sigma_a$  for materials that can be obtained from the measured values of  $\mu_m$  using the following relation, Eq. (3) [17]:

$$\sigma_a = \frac{\mu_m A_r}{N_A} \quad (3)$$

where  $N_A$  is the Avogadro's number ( $6.022045 \times 10^{23} \text{ mol}^{-1}$ ), and  $A_r$  is the relative atomic mass of the compound and is given by  $A_r = \frac{\sum_i n_i A_i}{\sum_i n_i}$ . The total electronic cross-section  $\sigma_e$  for the element is expressed by the following Eq. (4) [18]:

$$\sigma_e = \frac{1}{N_A} \sum_i \frac{f_i N_i}{Z_i} (\mu_m)_i = \frac{\sigma_a}{Z_{eff}} \quad (4)$$

where  $f_i$  denotes the fractional abundance of the element  $i$  with respect to the number of atoms,  $Z_i$  is the atomic number of the element  $i$ . Then, the effective atomic number  $Z_{eff}$  of the material can be defined as the ratio by Eq. (5):

$$Z_{eff} = \frac{\sigma_a}{\sigma_e} \quad (5)$$

Effective electron number or electron density  $N_{eff}$ , i.e., the number of electrons per unit mass, can be calculated through the Eq. (6):

$$N_{eff} = \frac{N_A}{N} Z_{eff} \sum n_i = \frac{\mu_m}{\sigma_e} \quad (6)$$

## Methods and materials

The values of the attenuation parameters were calculated in the energy range 10–60 keV for the investigated samples of natural raw and binderless *Rhizophora* spp. particleboards in four different particle sizes. The chemical composition and detailed information of the investigated samples are given elsewhere [12]. The binderless *Rhizophora* spp. particleboards were fabricated to obtain four different-sized particles with a target density of  $1 \text{ g/cm}^3$ . The particle sizes of the *Rhizophora* spp. samples are as follows: A ( $>147 \mu\text{m}$ ), B ( $147\text{--}74 \mu\text{m}$ ), C ( $74\text{--}50 \mu\text{m}$ ), and D ( $<50 \mu\text{m}$ ). Detailed information on the samples are shown elsewhere [11]. In addition, sample E is the *Rhizophora* spp. raw wood. The weight fractions of hydrogen, carbon, oxygen, and nitrogen in samples A, B, C, and D are 0%, 48.32%, 47.9%, and 3.78%, respectively. The weight fractions of the same elements in Sample E are 5.41%, 40.16%, 54.4%, and 0.03%, respectively. Finally, the maximum errors in the attenuation coefficients were calculated from the errors with different physical parameters associated with the present calculations; the estimated error of less than 4% was achieved.

MCNP5 is a general Monte Carlo code that can be used for neutron, photon, and electron or coupled neutron/photon/electron transport [19]. The MCNP5 input file simulates the experimental setup by using cell and surface cards in the input file. The MCNP5 output of the experimental setup is shown in Fig. 1. The photon mode is also considered in this simulation. The source (SDF) card was simulated to have a disk-shaped surface with 3 mm diameter and located 7 cm away from the end of the sample.

The elemental composition of the samples in the experimental setup was defined in the input file under the data cards. The detector shielding was designed in the form of a cylindrical lead collimator housing the detector with a diameter of 3 mm. The distances between (source–sample) and between (sample–detector) were 70 and 89 mm, respectively, as obtained experimentally by Marashdeh et al. [12]. The diameter of the samples was 1.34 cm. The transmitted beam of the photons was estimated for different

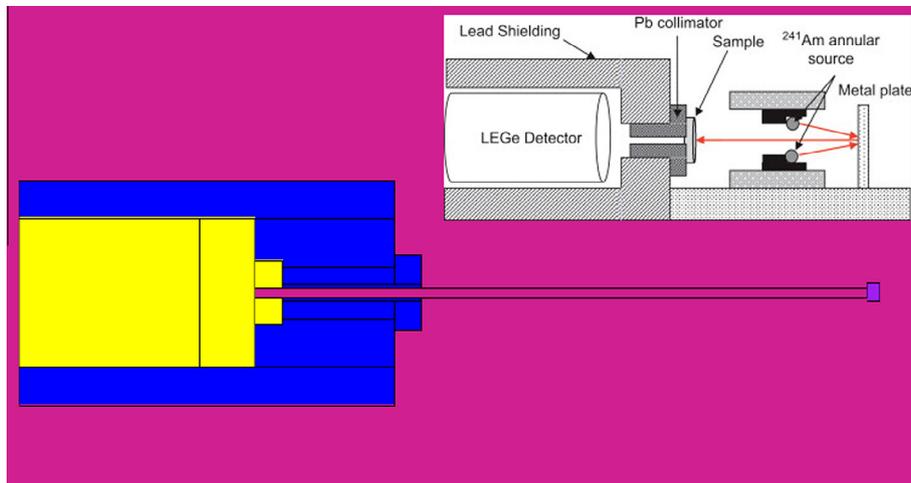


Fig. 1. The MCNP5 output of the experimental setup.

thicknesses of each sample (0.2–0.7 cm); then, the average value was calculated over these thicknesses. The linear attenuation for the samples at specified photon energy was determined using the output file value of the sample and an output file value without a sample to represent transmitted and incident gamma photon intensities respectively. The values were substituted into Eq. (1) to evaluate the linear attenuation coefficient of the sample. The code was repeated for different samples, and the simulation results were compared with the experimental results [12], and with the mass attenuation coefficient values determined by the XCOM program [20].

## Results and discussion

### Mass attenuation coefficient

The MCNP5 simulation code was employed to calculate the values of the mass attenuation coefficients ( $\mu_m$ ) for pure liquid water (Water 1), young-age breast tissue (Breast 1), and Aluminum (Al) over the photon energy range of 10–60 keV. The MCNP5 and the XCOM calculated values are plotted in Fig. 2. Relative differences of less than  $\pm 0.7\%$  were observed in the  $\mu_m$  values generated by

the two calculation methods, which validates the MCNP5 simulation method applied in this study. Similar findings were obtained by other workers (Medhat et al. [21] and Singh et al. [22]) validated the use of MCNP as an alternative method for XCOM to determine the mass attenuation coefficients for different composite materials at various energy ranges.

The MCNP5 code was then used to calculate the  $\mu_m$  values for the raw *Rhizophora* spp. wood (sample E) and the binderless *Rhizophora* spp. particleboards with different particle sizes (samples A, B, C, D) in the 10–60 keV energy regions. The MCNP5 calculations of the  $\mu_m$  values for *Rhizophora* spp. samples A to E are shown in Fig. 3. The values of  $\mu_m$  decreased sharply with energy, while the attenuation of photons also decreased with the increase in incident energy. This trend was observed for all curves regardless of particle size. Photoelectric absorption is the dominant interaction process for photon energy of less than 30 keV because of the importance of atomic binding. In this energy region, the  $\mu_m$  curves did not show absorption-edge discontinuities because the materials used have no high-Z constituents [23]. The contribution of the photoelectric absorption becomes negligible and the Compton scattering process dominates in the energy range of 30 keV and

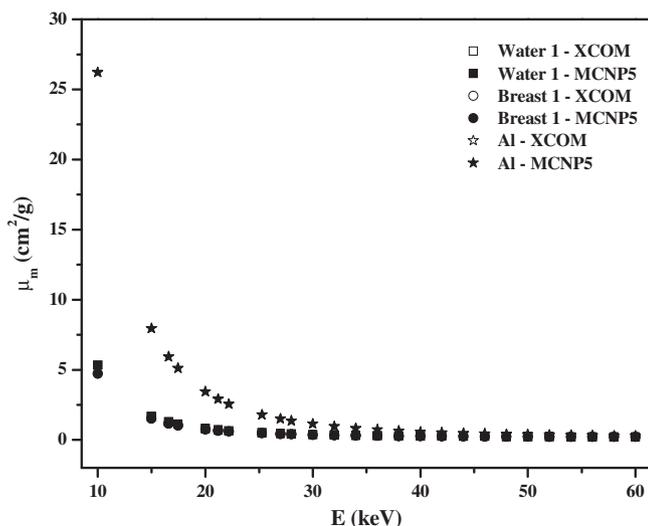


Fig. 2. A comparison of MCNP5 and XCOM calculated values of mass attenuation coefficients versus photon energy for water, breast and Al samples.

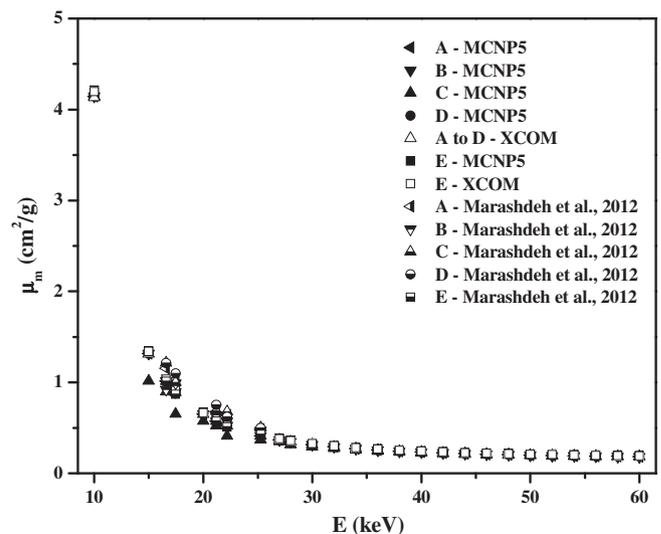


Fig. 3. A comparison of MCNP5 and XCOM calculated values as well as measured values of mass attenuation coefficients versus photon energy for *Rhizophora* spp. samples A to E.

above because the effective cross section is inversely proportional to the incident photon energy.

The  $\mu_m$  results for the *Rhizophora* spp. samples generated by the XCOM program in Fig. 3 shows that the MCNP5 generated values are in agreement with the corresponding XCOM calculated values. The relative differences in the  $\mu_m$  values between the two calculation methods are less than 0.6%, whereas no noticeable variations have been observed in the  $\mu_m$  values among the different binderless *Rhizophora* spp. particleboard samples. These results support the validity of the MCNP5 simulation code for the prescribed calculations and indicate that particle size has no effect on the attenuation of *Rhizophora* spp. wood for photon radiation. However, the figure reveals a slight difference in the attenuation of photons for the binderless *Rhizophora* spp. particleboards compared with that for raw wood, with relative differences in the  $\mu_m$  values of less than –4%. This discrepancy can be attributed to the differences in elemental composition between the two types of wood. Fig. 3 also shows the  $\mu_m$  coefficients for same samples (A, B, C, and E), as obtained experimentally by Marashdeh et al. [12] at energies between 16.59 and 25.26 keV. The MCNP5 calculations of the  $\mu_m$  values agree well with the measured values; thus, these findings unambiguously support the earlier conclusions [12].

The values of  $\mu_m$  for *Rhizophora* spp. samples were compared with those for water and breast samples by calculating their relative differences. The results are graphically depicted in Fig. 4. Noticeable variations in  $\mu_m$  values for the *Rhizophora* spp. samples are observed compared with those for Water 1 and Breast 1 samples, with average relative difference values of up to –15% and –11%, respectively. Fig. 4 also shows that the maximum relative difference in  $\mu_m$  values for the *Rhizophora* spp. samples compared with the Water 1 and Breast 1 samples is observed at 10 keV where the photoelectric absorption is dominant. This behavior can be attributed to the strong dependence of photoelectric absorption on atomic number [23] and the presence of higher atomic number

components (carbon and nitrogen) in *Rhizophora* spp. wood that do not exist in water. At 60 keV, where the Compton scattering is important, the relative differences in  $\mu_m$  values for the *Rhizophora* spp. samples compared with the Water 1 and Breast 1 samples is minimal because of the similar values of the electron density of the samples in this energy region, as presented below in the next section. Notably, the  $\mu_m$  values for the *Rhizophora* spp. samples are closer to those quoted for breast tissue than water as indicated in Fig. 4. This result agrees with the earlier findings obtained by Abuarra et al. [13]. Nevertheless, the noticeable discrepancies in  $\mu_m$  values compared with those of water and breast, strongly suggest that the elemental composition of *Rhizophora* spp. particleboard samples should be modified to obtain similar attenuation coefficients to water and breast tissue.

#### Effective atomic number and effective electron density

The total atomic cross-sections ( $\sigma_a$ ) for the investigated samples were calculated from the values of  $\mu_m$ , as previously described. The calculated  $\sigma_a$  values were compared against the theoretical  $\sigma_a$  values, as estimated using the XCOM program. A typical behavior of  $\sigma_a$  with photon energy for samples D and E is shown in Fig. 5. The  $\sigma_a$  values for Water 1 and Breast 1 samples are also included in the figure for validation and comparison. The values of  $\sigma_a$  calculated based on the MCNP5 code are in a very good agreement with those obtained theoretically. Meanwhile, the  $\sigma_a$  values for sample D are greater than those obtained for sample E, with relative differences of up to 60%, which is also attributed to the differences in elemental composition of samples. Afterward, the  $\sigma_e$  values were calculated to obtain the values of  $Z_{eff}$  and  $N_{eff}$  for all samples.

The calculated values of  $Z_{eff}$  for the investigated samples reveal the dependence of  $Z_{eff}$  on the elemental composition and relative proportions of the constituent elements. Thus, remarkable discrepancies were observed regarding the behavior of  $Z_{eff}$  values

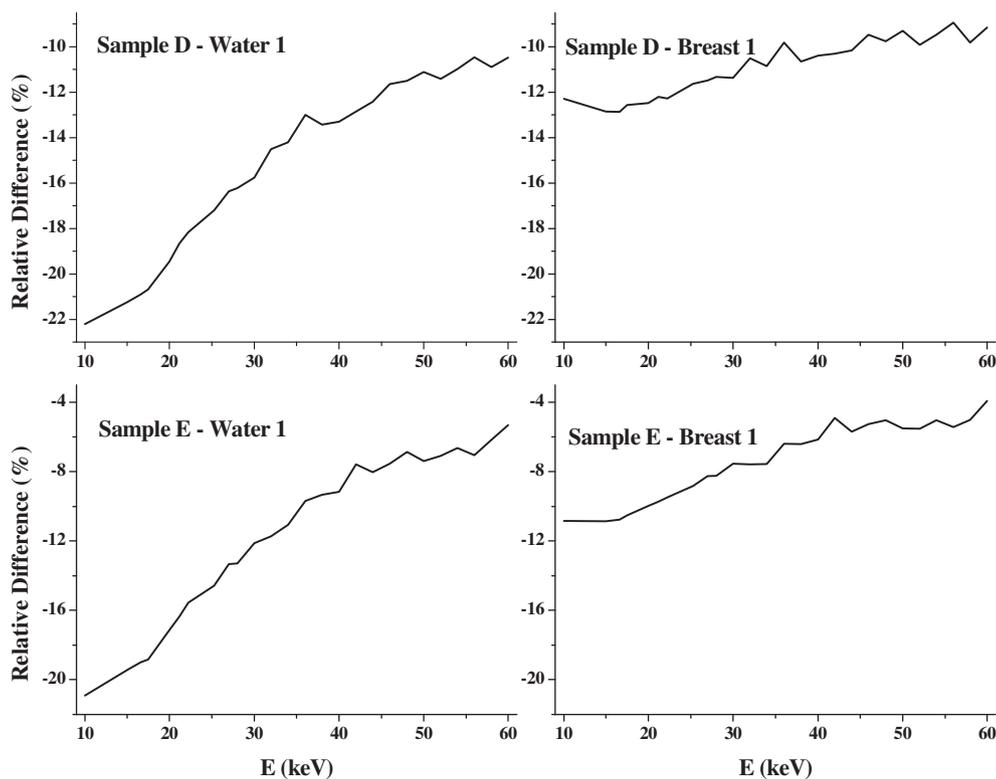


Fig. 4. Relative differences (%) in mass attenuation coefficients versus photon energy between water and breast samples, and *Rhizophora* spp. samples D and E.

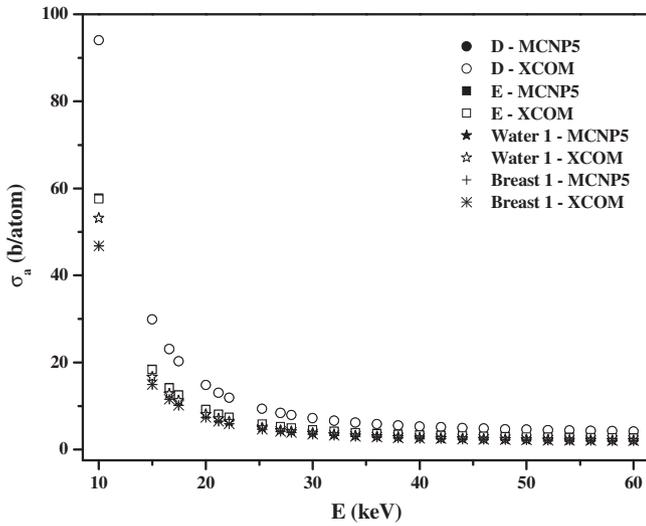


Fig. 5. Variation of total atomic cross section of samples D, E, Water 1 and Breast 1 with photon energy as obtained based on the MCNP5 and XCOM methods.

for each *Rhizophora* spp. sample with photon energy compared with those for water and breast samples. A typical variation of the  $Z_{eff}$  values for *Rhizophora* spp. samples D and E with photon energy is shown in Fig. 6, whereas the corresponding behavior of  $N_{eff}$  values is shown in the inset. In the case of variation of the  $\mu_m$  values, the variation of  $Z_{eff}$  and  $N_{eff}$  can be explained by the predominance of different processes of photon interaction in different energy regions. The main interaction in the low photon energy is photoelectric absorption; thus, maximum values of  $Z_{eff}$  and  $N_{eff}$  are obtained. Compton scattering is the main photon interaction when the photon energy increases; thus, the  $Z_{eff}$  and  $N_{eff}$  values are almost constant for the given samples. Moreover, Fig. 6 also shows that the  $Z_{eff}$  values for almost all of the samples lie within the range of 3.5–7.5. Worth to mention that Banjade et al. [10], have reported a value of  $Z_{eff}$  for *Rhizophora* spp. raw wood is 7.09, which matches our present result.

The effective atomic number is the most vital parameter in investigating the water and tissue equivalency of *Rhizophora* spp. [10,12,24]. In this regard, Fig. 6 clearly reveals that the variation

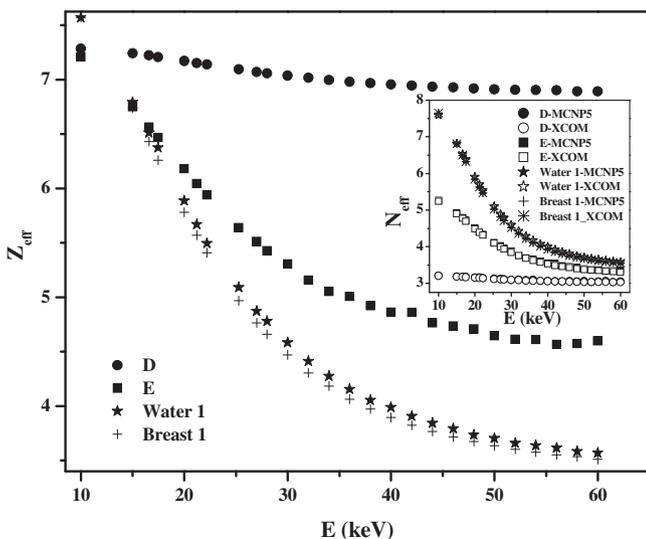


Fig. 6. Variation of effective atomic numbers of samples D, E, Water 1 and Breast 1 with photon energy as obtained based on the MCNP5 method. The inset shows the variation of effective electron density with photon energy for the same samples.

trend of the  $Z_{eff}$  values for raw wood is much closer to that of water and breast tissue than the binderless *Rhizophora* spp. particleboard samples. The four different particle sizes of binderless *Rhizophora* spp. particleboard (samples A, B, C, and D) show a slight variation in the  $Z_{eff}$  values over the photon energy used in this study, with minimum and maximum values of 7.3 and 6.9, respectively. However, this narrow range of variation in the  $Z_{eff}$  values for binderless *Rhizophora* spp. particleboards is expected and common among composites consisting of elements with close atomic numbers [24]. In the current case, the elements are C, N, and O. Therefore, the variation dependence of  $Z_{eff}$  for the binderless *Rhizophora* spp. particleboards significantly differs from those of water and breast tissue. This result implies that the equivalency parameters of binderless *Rhizophora* spp. particleboards with this particular composition do not match adequately with those of water or breast tissues. Meanwhile, Fig. 6 and its inset reveal that the variations of  $Z_{eff}$  and  $N_{eff}$  with the photon energy for all samples are similar because the two quantities are related by Eq. (5). Therefore, the relationship between  $Z_{eff}$  and  $N_{eff}$  is linear, as indicated in Fig. 7.

The mean atomic number of each compound investigated in this study was calculated from the chemical formula of the molecule  $\langle Z \rangle = \frac{1}{n} \sum_i n_i Z_i$ . The values of  $\langle Z \rangle$  for Water 1, Breast 1, samples A to D, and sample E were 3.33, 3.25, 6.85, and 4.33, respectively. A satisfactory agreement was found between the MCNP5 calculations of  $Z_{eff}$  and the  $\langle Z \rangle$  values in the upper energy region (60 keV) wherein the Compton scattering dominates. Therefore, in the energy region where the Compton scattering process is predominant, particularly for low Z compounds, the effective atomic number can be estimated by the mean atomic number, which is an average single-valued, composition-dependent but energy-independent number. This result is consistent with Sidhu et al. [25], who concluded that low Z composite materials can be represented by the energy independent and composite dependent mean atomic number  $\langle Z \rangle$ . However, the effective atomic number for the use of dosimetric or substitute materials should be evaluated for the energy range of interest and should not be assumed to be a constant. Such conclusions can also be verified using the XCOM software. Therefore, the values obtained by MCNP5, as well as the theoretical values of the  $Z_{eff}$  and  $N_{eff}$  for Water 1 and Breast 1 samples, are plotted against photon energy in Figs. 8a and 8b, respectively. Good agreement was achieved between the values of both calculation methods because the relative differences

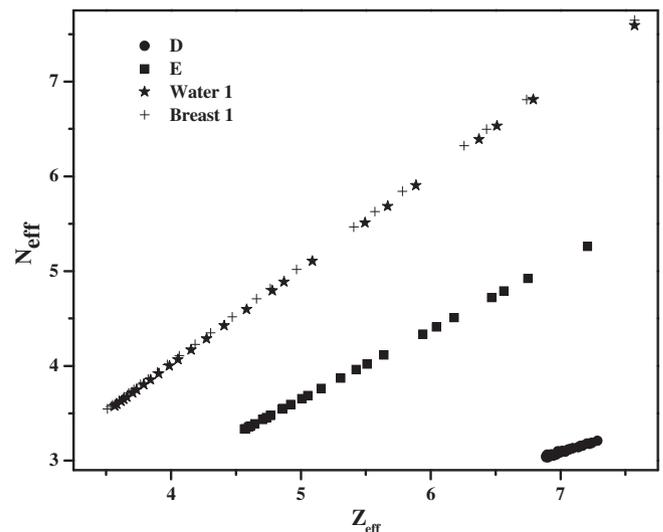
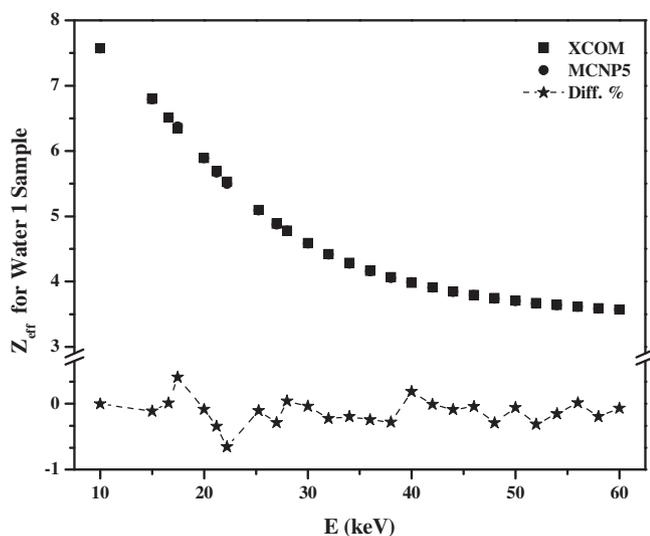
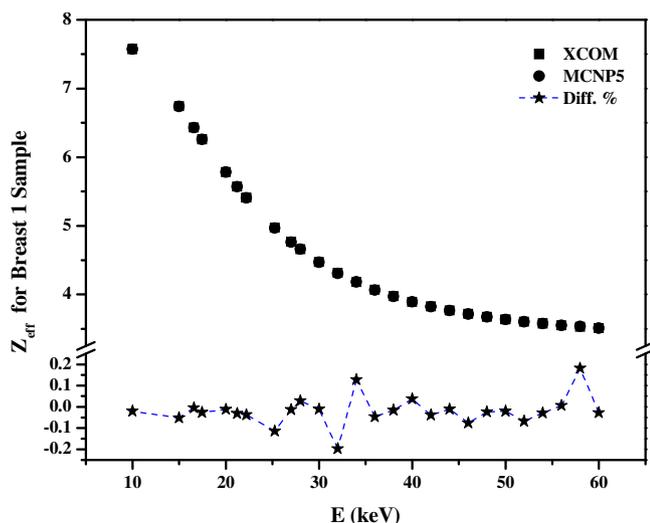


Fig. 7. Effective atomic numbers of samples D, E, Water 1 and Breast 1 versus effective electron density as obtained based on the MCNP5 method.



**Fig. 8a.** Variation of the effective atomic numbers for water with photon energy as obtained based on the MCNP5 and XCOM methods with the corresponding relative differences (%).



**Fig. 8b.** Variation of the effective atomic numbers for breast sample with photon energy as obtained based on the MCNP5 and XCOM methods with the corresponding relative differences (%).

between them were smaller than  $\pm 1\%$ . This consistency of the MCNP5 calculated values of  $Z_{eff}$  with the theoretically XCOM calculated values establishes the validity of the MCNP5 simulation for finding the  $Z_{eff}$  of such materials. Notably, the discrepancy is large in the low energy region where photoelectric effect is the predominant process, indicating that photoelectric absorption is strongly dependent on individual atomic numbers.

## Conclusion

In this study, the MCNP5 simulation code was applied to calculate the values of the mass attenuation coefficients ( $\mu_m$ ), total atomic cross section ( $\sigma_a$ ), effective atomic numbers ( $Z_{eff}$ ), and effective electron density ( $N_{eff}$ ) of *Rhizophora* spp. wood samples, as well as water and young-age breast tissue, over the energy range of 10 keV to 60 keV. The applicability of the MCNP5 code was satisfactory and in good agreement with the results generated by the XCOM program based on the mixture rule.

Therefore, all of these parameters are dependent on the incident photon energy, particularly in the low incident photon energies (1–30 keV) because of the predominant photoelectric absorption process. These parameters are nearly constant because of the predominance of the Compton scattering at  $\geq 30$  keV. In addition, the energy dependence of photon interaction cross section is identical to the total mass attenuation coefficient; the same can be concluded for the electron density and effective atomic number.

The binderless *Rhizophora* spp. particleboard samples exhibited attenuation parameters that significantly differ from those of Water 1 and Breast 1 samples, and thus do not match the water and tissue equivalency requirements. However, the raw wood of *Rhizophora* spp. is much closer to the breast tissue in terms of radiation interaction data. A satisfactory agreement between the calculated values of  $Z_{eff}$  and mean atomic number ( $Z$ ) of *Rhizophora* spp. wood is found in the 30–60 keV energy region. Therefore, this energy-independent and composition-dependent parameter of low-Z composite materials can be a good estimate of the effective atomic number in the energy region wherein Compton scattering is predominant.

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