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Original Article

Monte Carlo approach for calculation of mass energy absorption coefficients of some amino acids

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ABSTRACT

This study offers a Monte Carlo alternative for computing mass energy absorption coefficients of any material through calculation of photon energy deposited per mass of the sample and the energy flux obtained inside a sample volume. This approach is applied in this study to evaluate mass energy absorption coefficients of some amino acids found in human body at twenty-eight different photon energies between 10 keV and 20 MeV. The simulations involved a pencil beam source modeled to emit a parallel beam of mono-energetic photons toward a 1 mean free path thick sample of rectangular parallelepiped geometry. All the components in the problem geometry were surrounded by a 100 cm vacuum sphere to avoid any interactions in materials other than the absorber itself. The results computed using the Monte Carlo radiation transport packages MCNP6.2 and GAMOS5.1 were checked against the theoretical values available from the tables of XMUDAT database. These comparisons indicate very good agreement and support the conclusion that Monte Carlo technique utilized in this fashion may be used as a computational tool for determining the mass energy absorption coefficients of any material whose data are not available in the literature.

1. Introduction

Due to being a penetrating type of radiation, photons are extensively utilized in medical and industrial settings to irradiate materials for applications like imaging, treatment, measurements, sterilization, etc. They are indirectly ionizing radiations which may transfer part of their energy to the electrons of atoms and molecules in materials through which they pass and they produce ionization and excitation interactions in this process. As a result, certain radiation effects are observed to develop in all materials.

The extent of irradiation by photons is usually tackled by using a quantity called attenuation coefficient which is defined for mono-energetic particles and narrow beams. This quantity is usually used as linear attenuation coefficient (denoted as μ and expressed in units of cm^{-1}) or mass attenuation coefficient (μ/ρ, in units of cm^2/g) to eliminate any dependence on density or physical state of the material. It corresponds to the probability for a photon to undergo scatter or absorption interactions per unit distance of an absorber and is usually employed to identify the material's attenuation capability (absorption plus scattering) against all photons of a specific energy. A comprehensive review of the available studies that report mass attenuation coefficients for various materials in a wide range of photon energies can be found in Ref. [1].

Although μ/ρ may be taken as a tool for a rough estimate of thickness of a material to shield a known type and energy of an ionizing photon beam, it does not yield much information regarding any radiation effects produced in materials being irradiated. In case of biological entities, the harmful effects that may happen after energy deposition are known to damage the integrity and activity of cells in tissues [2]. The severity of these may be associated with the properties of the absorbing material and as well as the dose it absorbs, which is defined as the energy deposited per unit mass. There is another quantity known as mass energy absorption coefficient (μ_{en}/ρ) [3] used in radiation dosimetry to account for the mean energy of the incident photons absorbed in the absorber. μ_{en}/ρ is considered a significant tool in medical and health physics and provides valuable information for estimating absorbed dose since the energy transferred to the charged particles as kinetic energy from photon interactions is the main reason for radiation effects induced in a material medium [4]. There is an online

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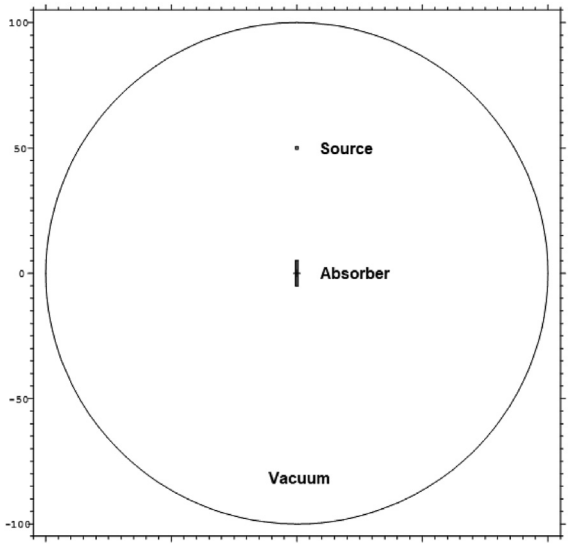


Fig. 1. Geometrical view of the model setup taken from MCNP's plotting interface.

Table 1
Some properties of the amino acids investigated in this study.

Amino Acid	Chemical formula	M (g/mol)
Alanine	$C_3H_7NO_2$	89.093
Arginine	$C_6H_{14}N_4O_2$	174.201
Asparagine	$C_4H_8N_2O_3$	132.118
Aspartic Acid	$C_4H_7NO_4$	133.103
Cysteine	$C_3H_7NO_2S$	121.159
Glutamic Acid	$C_5H_9NO_4$	147.129
Glutamine	$C_5H_{10}N_2O_3$	146.145
Glycine	$C_2H_5NO_2$	75.067
Histidine	$C_6H_9N_3O_2$	155.155
Leucine	$C_6H_{13}NO_2$	131.173
L-Lysine	$C_6H_{14}N_2O_2$	146.188
L-Serine	$C_3H_7NO_3$	105.093
L-Tryptophan	$C_{11}H_{12}N_2O_2$	204.225
Methionine	$C_5H_{11}NO_2S$	149.212
Phenylalanine	$C_9H_{11}NO_2$	165.189
Proline	$C_5H_9NO_2$	115.130
Threonine	$C_4H_9NO_3$	119.119
Tyrosine	$C_9H_{11}NO_3$	181.189
Valine	$C_5H_{11}NO_2$	117.146

database that provides tabular data as well as a software for obtaining mass energy absorption coefficient for many elements, compounds or mixtures [3]. In addition, literature studies are mostly limited to experimental or computational reports of mass attenuation coefficients of various absorber materials [4–15]. There are very few papers in literature on mass energy absorption coefficients, most of which are based on XMUDAT data [16]. For organic materials that are biologically significant, such as carbohydrates, amino acids, fatty acids and proteins, there is a scarce amount of data. One can of course take the elemental composition and the individual μ_{en}/ρ values from the tables and apply the additivity rule to find μ_{en}/ρ of any material whose data are not available from this database. This, however, brings some degree of error as mentioned by Attix [4].

A better method to directly devise a formulation for finding mass energy absorption coefficient of a material can be using a calculational procedure such as the Monte Carlo method. This study proposes this procedure as an alternative for computing μ_{en}/ρ of some amino acids found in human body. The calculations employ simulations carried out in a wide range of photon energies that are encountered in dosimetric situations and compare the investigated μ_{en}/ρ values with the data produced from XMUDAT tables [16].

2. Material and method

Monte Carlo method is a statistical method widely used in many different fields of science and engineering when analytical or numerical solutions are difficult, if now impossible, to obtain. The technique utilizes pseudo-random numbers from a computer algorithm in association with certain probability distributions to search for an average of a physical quantity in question. It is very well tested in radiation transport problems because photon interactions with matter may be described on the basis of microscopic cross-sections which themselves are described as probabilistic quantities that depend on beam parameters and elemental compositions. In photon transport problems, a Monte Carlo code provides computational estimates of such dosimetric quantities as flux, energy deposition, dose, etc. based on these interaction cross sections [17] based on the geometrical and material descriptions of the medium of interaction.

In this study, two Monte Carlo software packages, namely MCNP 6.2 and GAMOS 5.1, were employed for modeling the geometry of the source, the absorber and the detector as well as estimating the

Table 2
Total mass energy absorption coefficients (cm^2/g) of amino acids at various photon energies determined by MCNP simulations.

Energy (MeV)	Alanine	Arginine	Asparagine	Aspartic A.	Cysteine	Glutamic A.	Glutamine
0.01	3.394	3.021	3.528	3.8	15.52	3.605	3.36
0.015	0.9393	0.8334	0.9763	1.053	4.641	0.9982	0.9291
0.02	0.3776	0.3346	0.3921	0.423	1.943	0.4013	0.3732
0.03	0.1099	0.09799	0.1136	0.1222	0.5678	0.1163	0.1087
0.04	0.05142	0.04672	0.05276	0.05604	0.2409	0.05386	0.05087
0.05	0.03333	0.03104	0.03389	0.03542	0.128	0.03437	0.03297
0.06	0.02672	0.02548	0.02688	0.02766	0.08037	0.02716	0.02646
0.08	0.02351	0.02305	0.02337	0.02358	0.04508	0.02348	0.02329
0.1	0.02379	0.02357	0.02352	0.02355	0.03427	0.02359	0.02358
0.15	0.0264	0.02637	0.02602	0.0259	0.02899	0.02604	0.02617
0.2	0.02854	0.02856	0.02812	0.02794	0.02929	0.02813	0.0283
0.3	0.03085	0.03088	0.03037	0.03018	0.03063	0.03038	0.03058
0.4	0.03176	0.03181	0.03126	0.03105	0.03132	0.03128	0.03149
0.5	0.03198	0.03202	0.03147	0.03127	0.03146	0.03149	0.0317
0.6	0.03185	0.03189	0.03134	0.03113	0.03129	0.03136	0.03157
0.8	0.03109	0.03113	0.03059	0.03038	0.03051	0.0306	0.03081
1	0.03011	0.03015	0.02962	0.02942	0.02954	0.02964	0.02984
1.25	0.02878	0.02883	0.02833	0.02814	0.02824	0.02834	0.02854

(*continued on next page*)

Table 2 (*continued*)

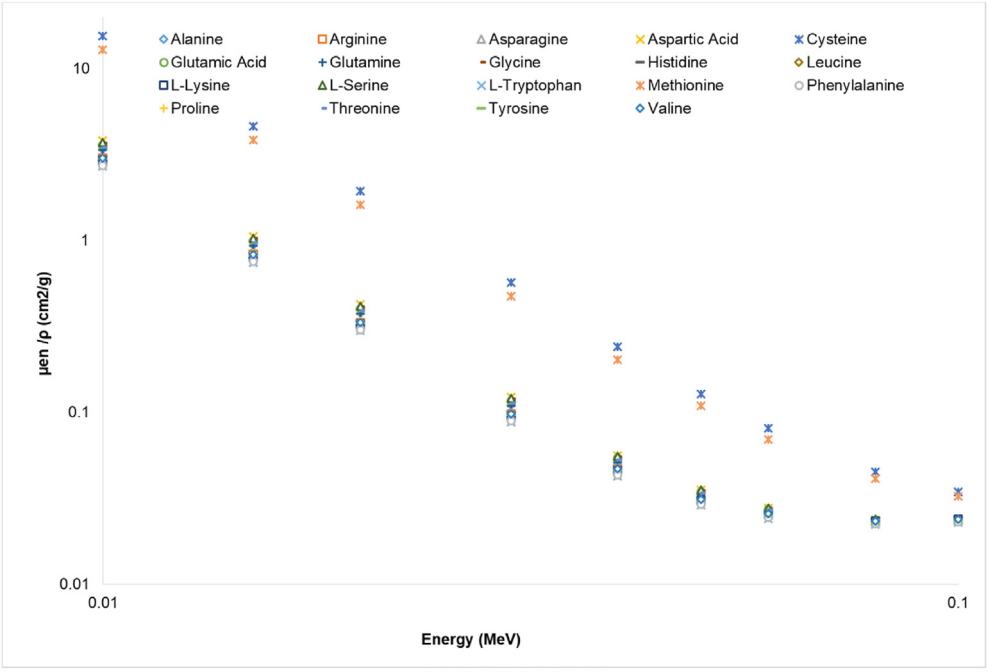
Energy (MeV)	Alanine	Arginine	Asparagine	Aspartic A.	Cysteine	Glutamic A.	Glutamine
1.5	0.0275	0.02754	0.02706	0.02688	0.02698	0.02707	0.02727
2	0.0253	0.02534	0.0249	0.02473	0.02486	0.0249	0.02507
3	0.02209	0.02211	0.02176	0.02163	0.0219	0.02177	0.02191
4	0.01998	0.01997	0.01971	0.0196	0.02003	0.01971	0.01981
5	0.0185	0.01847	0.01827	0.01819	0.01875	0.01826	0.01836
6	0.01741	0.01736	0.0172	0.01714	0.01785	0.01721	0.01727
8	0.01595	0.0159	0.0158	0.01578	0.01672	0.01582	0.01585
10	0.01504	0.01495	0.01492	0.01492	0.01606	0.01494	0.01495
15	0.01379	0.01368	0.01374	0.01378	0.01527	0.01375	0.01372
20	0.01322	0.01307	0.0132	0.01327	0.01496	0.01322	0.01316

Energy (MeV)	Glycine	Histidine	Leucine	L-Lysine	L-Serine	L-Tryptophan
0.01	3.7	3.07	2.876	2.919	3.727	2.701
0.015	1.025	0.8468	0.795	0.8062	1.033	0.7435
0.02	0.4118	0.34	0.3193	0.324	0.415	0.2982
0.03	0.1192	0.0992	0.09402	0.09518	0.1202	0.08786
0.04	0.055	0.04703	0.04537	0.04583	0.05539	0.04252
0.05	0.035	0.03103	0.03054	0.03073	0.03517	0.0289
0.06	0.02755	0.0253	0.02534	0.0254	0.02764	0.02412
0.08	0.02371	0.02269	0.02316	0.02315	0.02375	0.02222
0.1	0.02377	0.02315	0.02385	0.02381	0.02379	0.02294
0.15	0.02621	0.02585	0.02678	0.02671	0.02621	0.02581
0.2	0.0283	0.02799	0.02902	0.02893	0.0283	0.02798
0.3	0.03057	0.03025	0.03139	0.03129	0.03057	0.03027
0.4	0.03145	0.03116	0.03232	0.03222	0.03145	0.03116
0.5	0.03167	0.03136	0.03255	0.03244	0.03167	0.03137
0.6	0.03153	0.03124	0.03241	0.03231	0.03154	0.03124
0.8	0.03077	0.03049	0.03165	0.03154	0.03078	0.0305
1	0.02981	0.02953	0.03065	0.03055	0.0298	0.02955
1.25	0.02851	0.02823	0.02931	0.02921	0.02851	0.02825
1.5	0.02723	0.02697	0.02801	0.02791	0.02723	0.02699
2	0.02506	0.02481	0.02577	0.02569	0.02506	0.02482
3	0.0219	0.02167	0.02246	0.0224	0.02191	0.02166
4	0.01984	0.0196	0.02028	0.02023	0.01984	0.01958
5	0.01838	0.01814	0.01874	0.0187	0.01839	0.0181
6	0.01732	0.01707	0.01759	0.01755	0.01732	0.017
8	0.01592	0.01565	0.01605	0.01603	0.01593	0.01556
10	0.01504	0.01476	0.01508	0.01506	0.01504	0.01464
15	0.01385	0.01354	0.01373	0.01373	0.01386	0.01339
20	0.01331	0.01298	0.01309	0.01309	0.01332	0.01279

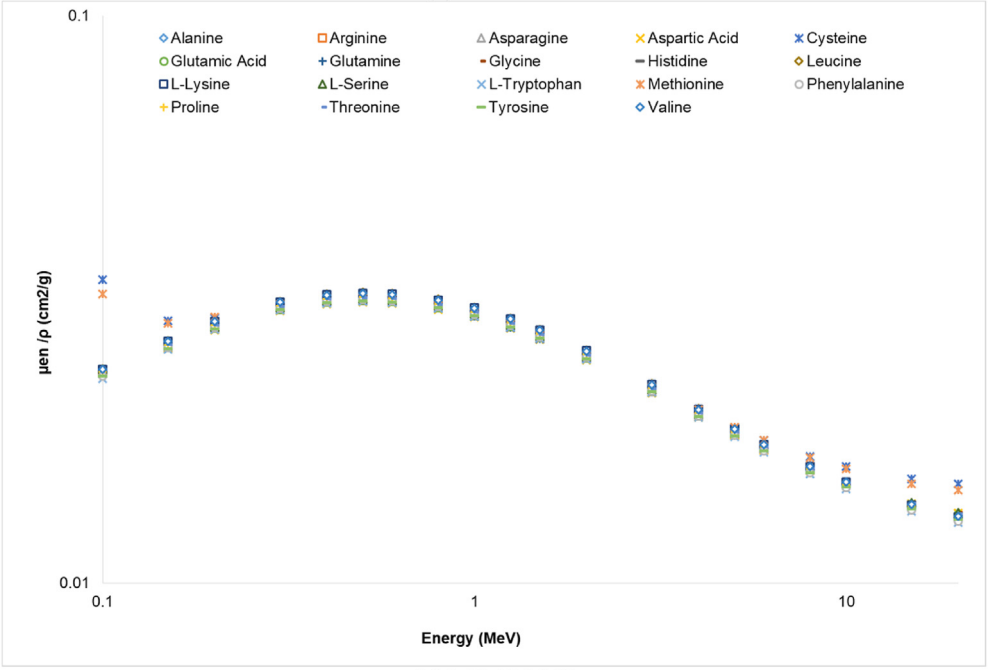
Energy (MeV)	Methionine	Phenylalanine	Proline	Threonine	Tyrosine	Valine
0.01	12.92	2.739	3.058	3.492	2.987	3.008
0.015	3.855	0.7541	0.8457	0.9678	0.8244	0.8314
0.02	1.614	0.3027	0.3398	0.3893	0.3307	0.334
0.03	0.473	0.08925	0.09946	0.113	0.09687	0.09806
0.04	0.2019	0.04308	0.04733	0.0527	0.04613	0.04688
0.05	0.1089	0.02919	0.03131	0.0339	0.0306	0.03121
0.06	0.06951	0.02435	0.02558	0.027	0.02508	0.02567
0.08	0.04087	0.02242	0.02302	0.02356	0.02262	0.02326
0.1	0.03235	0.02313	0.02355	0.02378	0.02316	0.02383
0.15	0.0287	0.026	0.02631	0.02635	0.0259	0.0267
0.2	0.02941	0.02818	0.02848	0.02847	0.02805	0.02891
0.3	0.03099	0.03049	0.03081	0.03076	0.03033	0.03127
0.4	0.03173	0.03139	0.03172	0.03167	0.03122	0.03219
0.5	0.03188	0.03161	0.03193	0.03188	0.03144	0.03241
0.6	0.03171	0.03147	0.0318	0.03175	0.03131	0.03229
0.8	0.03093	0.03073	0.03105	0.03099	0.03056	0.03151
1	0.02995	0.02976	0.03007	0.03002	0.0296	0.03052
1.25	0.02863	0.02846	0.02875	0.0287	0.0283	0.02919
1.5	0.02736	0.02719	0.02748	0.02742	0.02704	0.02789
2	0.0252	0.025	0.02529	0.02523	0.02487	0.02564
3	0.02214	0.02182	0.02206	0.02204	0.02172	0.02237
4	0.02018	0.01971	0.01994	0.01994	0.01964	0.02021
5	0.01883	0.01823	0.01845	0.01847	0.01817	0.01868
6	0.01786	0.01711	0.01734	0.01738	0.01709	0.01753
8	0.01663	0.01565	0.01587	0.01594	0.01566	0.01603
10	0.01589	0.01472	0.01493	0.01504	0.01475	0.01506
15	0.01494	0.01345	0.01366	0.01381	0.01351	0.01374
20	0.01456	0.01285	0.01306	0.01324	0.01293	0.01311

interactions of photons with atoms and their detection at a point of interest. MCNP6 is a general-purpose radiation transport package developed in Los Alamos National Laboratory [18]. It is capable of transporting many different types of source particles in three-dimensional geometries and handling various types of detectors for recording particle contributions. GAMOS, on the other hand, is a variant of Geant4 developed by CERN [19] and is widely used by medical physicists to study ionizing radiation sources in diagnostic or treatment applications [20]. MCNP comes with ENDF/B VII cross section packages to estimate particle interactions while GAMOS uses physics packages to treat different types of source particles in a wide energy range and to score for desired particle properties.

The simulations involved a pencil beam photon source placed in a 1-cm vacuum cube which emits a mono-energetic and photon beam directed toward the rectangular parallelepiped absorber (cross-sectional edges being 1 cm; thickness = 1 mean free path) positioned 50 cm away from the source. In this configuration, the absorber also serves as the detector for energy absorption and flux scoring. All the components of the irradiation geometry were placed inside a vacuum sphere (r = 100 cm) to avoid any interactions of photons inside materials other than the sample. Fig. 1 depicts the irradiation setup obtained from MCNP plot module.



(a) 0.010-0.1 MeV



(b) 0.10-20 MeV

Fig. 2. Mass energy absorption coefficients (cm^2/g) of amino acids as a function of photon energy obtained from MCNP simulations.

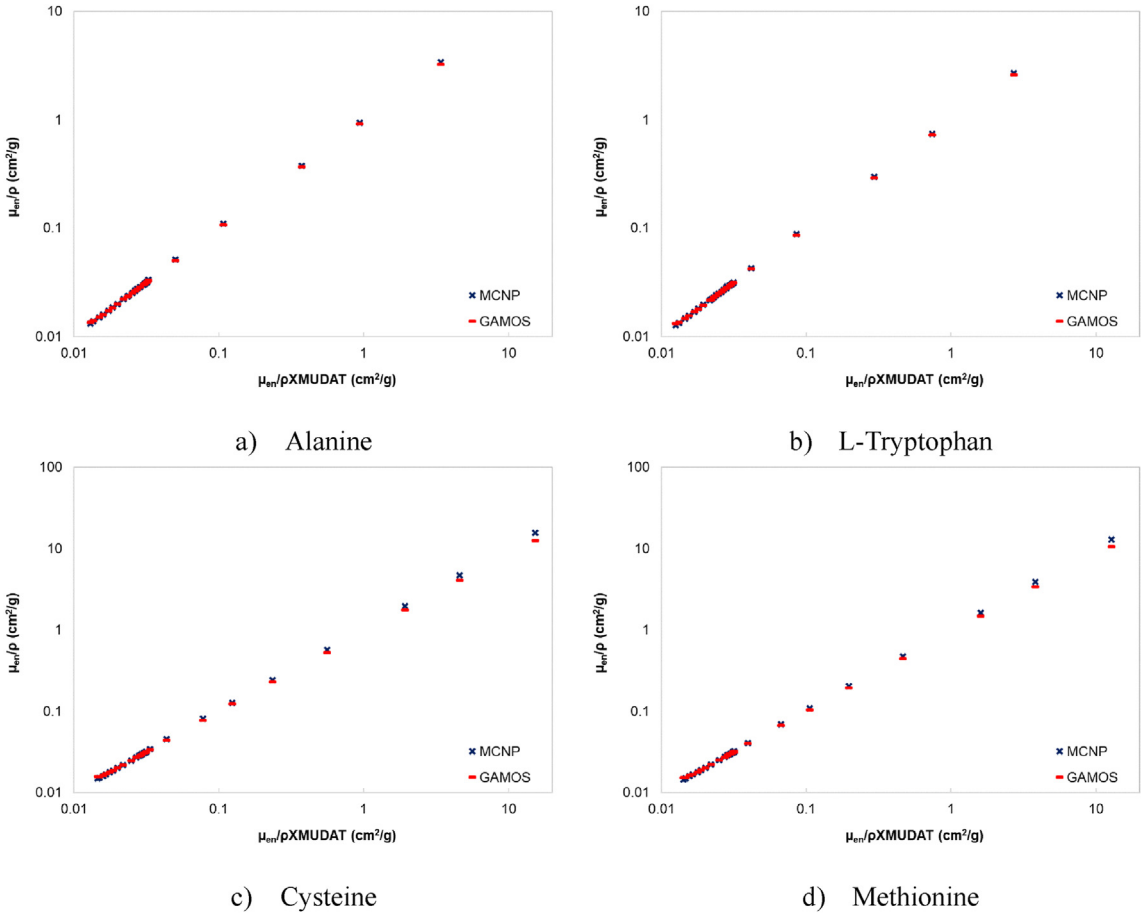


Fig. 3. Mass energy absorption coefficients (μ_{en}/ρ) of some of the amino acids obtained from Monte Carlo simulations (MCNP and GAMOS) plotted against data from XMUDAT database [16].

In this paper, nineteen different amino acids that were deemed to be significant in biological systems were investigated for photon absorption. Table 1 provides chemical formula and molecular mass of each of the sample. From a radiation interaction perspective, they basically differ from one another by the varying proportion of the elements H, C, N, O or S. From the chemical formulae and atomic weights provided, the percent fractions of individual elements in each sample were calculated and inserted into Monte Carlo simulations as elemental composition information.

For each of the sample, photon energies in the range 10 keV–20 MeV were investigated, each representing a different simulation. All the Monte Carlo runs were carried out with 10^6 particle histories/tracks which provided statistical errors that were less than 0.1% both in MCNP and GAMOS simulations which took, on the average, a few minutes to complete on a Intel Xeon 2.1 GHz with 64 GB ram memory. No variance reduction technique was employed in the simulations.

In estimating interaction properties of photons, energy flux and energy deposition features of each code were utilized which return an average of the total energy flux (Φ_E in MeV/cm^2) and energy deposition (E_{dep} in MeV), respectively, recorded in the absorber. The ratio of E_{dep} and Φ_E were then calculated for each sample at the energies considered to obtain the corresponding mass energy absorption coefficients.

3. Results and discussion

Mass energy absorption coefficients of nineteen amino acids were evaluated using the Monte Carlo method at twenty-eight different photon energies between 10 keV and 20 MeV. For each simulation, energy flux and energy deposition values were computed by the Monte Carlo codes to finally obtain μ_{en}/ρ results. Table 2 presents the data obtained from only one of these codes (MCNP) since the data produced by MCNP and GAMOS were very similar within statistical errors.

As expected, μ_{en}/ρ values of all the samples first exhibit a sharp decrease as a function of energy up to about 100 keV depending on the effective atomic number of the absorber as displayed in Fig. 2(a) and (b). The samples with higher atomic numbers have higher mass energy absorption coefficients as shown by the amino acids methionine and cystine which contain some amount of sulfur in addition to H, C, N and O. This behavior is a direct result of the photoelectric absorption being the dominant mode of interaction in this energy interval. After this initial sudden decrease, μ_{en}/ρ values observe a slow increase followed by a gradual decrease dictated by photon energy where all the samples follow an almost similar trend with little or no Z dependence. This latter behavior, on the other hand, may be attributed to Compton scattering being more significant at intermediate and higher energies. In this energy region where the incoming photons leave the interaction site with considerable amount of energy, the probability for energy absorption seems to increase with photon energy up to sufficiently higher energies of MeV level after which the effect of atomic number becomes significant again.

The majority of the MCNP and GAMOS results investigated in this study were observed to agree with each other within <0.5%

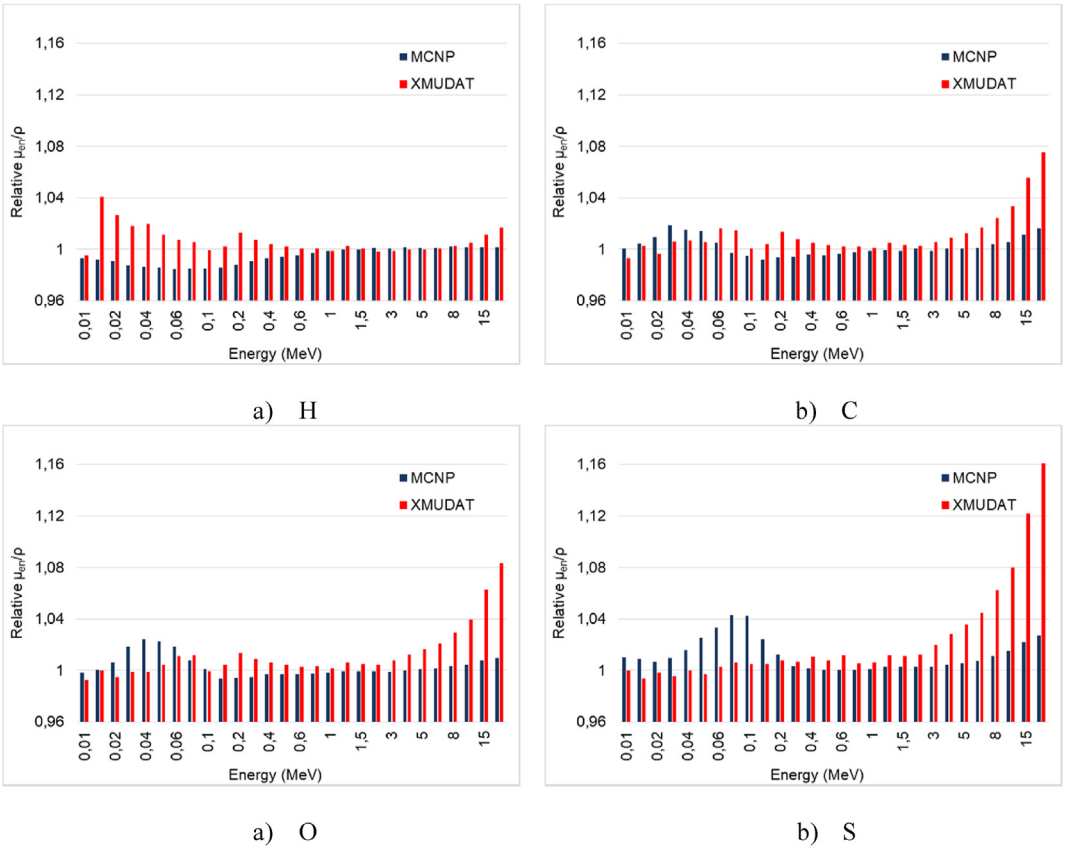


Fig. 4. μ_{en}/ρ values of MCNP and XMUDAT divided by those of NIST for the constituent elements of the amino acids [3,16].

which is a proof that the simulation configurations and the physics parameters employed in both codes were rather similar. When the results of each code were compared with those of XMUDAT tables [16], MCNP was seen to produce results agreeing within <0.5% while the percentage difference of GAMOS results were only slightly higher. The corresponding R^2 values of the correlations were exactly one in both comparisons which indicate a very satisfactory agreement between the simulation results and the corresponding tabular data. Fig. 3 compares results of MCNP and GAMOS with data from XMUDAT compilations for four of the samples where some discrepancy is observed at lower energies (less than 3% below 60 keV) and high energies (about 1% above 15 MeV). To understand the cause of these deviations, μ_{en}/ρ values of the ingredient elements (namely H, C, O and S) at the same energies obtained from MCNP and XMUDAT software were compared against online NIST tables. This disagreement is pronounced in Fig. 4a for μ_{en}/ρ of hydrogen at lower energies where as much as 4% difference is observed between XMUDAT and NIST. Fig. 4b–d, on the other hand, explain the disagreement at high energies in terms of the constituent elements of relatively higher atomic number (C, O, and S). Monte Carlo results show much better agreements at other energies.

4. Conclusion

In this study, a Monte Carlo approach for computing mass energy absorption coefficients of any material is proposed through calculations of such quantities as energy deposition and energy flux obtained inside a sample volume. This can be a valuable computational tool for samples and energies of interest for which there are limited data. In order to prove the feasibility of this approach, mass energy absorption coefficients of some amino acids found in human body were evaluated at some photon energies and the simulation results were checked against the theoretical values of XMUDAT database. The comparisons indicated very good overall agreement as a result of which we can assert that by utilizing Monte Carlo simulations in this fashion we can compute mass energy absorption coefficients of any material whose data are not available in the literature.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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