Decomposition of a tissue into its constituent elements for specifying the values of doses

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Abstract: - In this research, a real tissue has been decomposed to its constituent materials and elements applying its volumetric density and initial mass. This study has been carried out to obtain the exact amounts of constituent elements existing in liver tissue as well as specify the absorbed dose because of the tissue getting exposed to radiation in radiotherapy and radiography. In order, a medical model has been defined in a way that its compositions are just like the materials existing in the tissue of a human. Then, the accurate mass, density, and volume of every element in it are specified. In the next stage, the related tissue is exposed to a neutron beam, and then the values of doses absorbed in the main constituent material namely water, and also the total absorbed dose is obtained by the MCNP nuclear code. This study can be used to study the radiotherapy and radiography scopes for obtaining the absorbed dose as a result of interaction between radiation beam and biological cells. In this research, the values of absorbed doses have been obtained for a wide range of neutron energies in a way that the absorbed doses can accurately be obtained.

Key-Words: - Constituent elements; Dose; Radiation; Tissue.

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1 Introduction

In this investigation, the thickness of adipose tissue, which has been considered for the simulation, is 30 mm [1, 2]. One of the

compositions of adipose tissue is fat. The chemical formula of fat is CH2ORCHOR'CH2OR. Fat is not a compound. It is a mixture of many esterified acids named: fatty acids. The average skin thickness is thicker in males than females. The average pure skin thickness in males is average 1.5 mm. The skin tissue and subcutaneous consist of some portions such as the epidermis, dermis, hypodermis, and fat [3]. Skin is not a single substance, so it doesn't have a single formula. It has largely been made of various proteins, water, fat, and salt. Skin is a biological tissue that consists of carbon, oxygen, and nitrogen [4].

2 Materials and Methods

The correct representations of the geometry and compositions of tissues, which are in front of the liver tissue, have also accurately been considered concerning an adult male liver tissue for this study. Since, in this study, the calculation method and simulation of tissues may slight difficult be to understand, to better explain, all calculations regarding tissues, which are in front of the liver tissue, are expressed as below:

The distance from the body surface (nearest section into the body for setting the neutron source) to the liver is averagely considered 3 cm for a normal body. If the diameter of the neutron source head is 3 cm, then the path, where the neutron beam crosses to reach the liver, will almost be a cylinder with r=1.5 cm and h \approx 3 cm the volume of it will be: 21.20 cm3. This path plays the role of the collimator to reach the neutron beam from the source. According to the calculated volume and density of adipose (0.905 g/cm3), the mass of adipose existing in the mentioned path will be:

 $m = \rho \times V = 0.905 \times 21.20 = 19.18g$

According to the percentage of water, fat, and protein in adipose, the mass of them (in this volume of adipose) will be respectively:

For water:
$$\frac{10.2}{100} \times 19.18 = 1.95 \text{ g} (\text{H}_2\text{O})$$

For fat: $\frac{87.2}{100} \times 19.18 = 16.72 \text{ g}$
(CH₂ORCHOR'CH₂OR)

For protein:
$$\frac{2.1}{100} \times 19.18 = 0.40$$
 g
(C₄₄₁₈₉H₇₁₂₅₂N₁₂₄₂₈O₁₄₀₀₇S₃₂₁)

The spatial average of the protein density can be considered equivalent to 1.35 g/cm3, independent of the nature of the protein and particularly independent of its molecular weight. The density of human body fat is also: 0.918 g/cm3 [5, 6, 7].

Therefore, both the total density and volume of materials existing in the mentioned path, which is in front of the liver tissue, are calculated as below:

$$\begin{split} \rho_{Total} &= \frac{m_{Total}}{\frac{m_{Water}}{\rho_{Water}} + \frac{m_{Fat}}{\rho_{Fat}} + \frac{m_{Protein}}{\rho_{Protein}}} = \frac{1.95 + 16.72 + 0.40}{\frac{1.95}{1} + \frac{16.72}{0.918} + \frac{0.40}{1.35}} = \\ \frac{19.07}{1.95 + 18.21 + 0.29} &= \frac{19.07}{20.45} = 0.93 \, gr \, / \, cm^3 \\ V_{Total} &= \frac{m_{Total}}{\rho_{Total}} = \frac{19.07}{0.93} = 20.5 \, cm^3 \rightarrow \\ \pi \times (r_2^2 - r_1^2) \times h = 20.5 \, cm^3 \end{split}$$

Where:

 $r_1=1.5$ cm (radius of neutron source head), $h\approx 3$ cm (distance between body surface and liver)

Therefore:

$$\pi \times (r_2^2 - 2.25) \times 3 = 20.5 \rightarrow r_2 = 2.10cm$$

Thus, in this modelling, the path, where the neutron beam passes across it to reach the liver tissue, is considered a cylinder that has an inside radius of $r_1=1.5$ cm and an outside radius of $r_2=2.10$ cm [8, 9, 10].

The mass, thickness, and outside radius of every layer and shell have accurately been calculated. It meets actual dimensions, from which calculation of various layers is filled up with them.

(I)

i) Since in this study a sample liver weighing 2kg (for an adult male) has been considered, therefore:

ii) The weight of water existing in the mentioned tissue will be [11, 12, 13]:

$$\frac{69.69}{100}$$
 × 2000 = 1393.8 g (Water)

iii) Therefore, the weight of existent hydrogen in water is:

$$\frac{2.016}{18.015} \times 1393.8 = 155.975 \text{ g (H)}$$

iv) Similarly, the weight of existent oxygen is also calculated as below:

$$\frac{15.999}{18.015} \times 1393.8 = 1237.824 \text{ g (O)}$$

(II)

i) Then, a similar calculation is carried out for glycogen existing in the sample liver [14, 15, 16]. The weight of 1 gram-molecular of glycogen (C24H42O21) \rightarrow 288.264 (C) + 42.336 (H) + 335.979 (O) =666.579 g

ii) The weight of glycogen existing in the mentioned tissue will be:

$$\frac{0.35}{100} \times 2000 = 7 \,\mathrm{g} \,\mathrm{(Glycogen)}$$

iii) Therefore, the weight of existent carbon in glycogen is: $\frac{288.264}{666.579} \times 7 = 3.027$ g (C)

iv) Similarly, the weight of existent hydrogen and oxygen are also calculated as below:

For hydrogen:
$$\frac{42.336}{666.579} \times 7 = 0.444$$
 g (H)

For oxygen:
$$\frac{335.979}{666.579} \times 7 = 3.528 \text{ g (O)}$$

(III)

i) As two of the compositions of the liver tissue are protein and glucose, the molecules of each of them are decomposed to the related constituent elements, and taking the molecule gram into consideration, the amount of each atom existing in a molecule is extracted based on the number of atoms and the composition percentage of protein and glucose, which are alike 29.9% of the liver tissue.

Thus, a similar calculation is carried out for protein and glucose existing in the sample tissue. Due to the same percentage of protein and glucose existing in the liver (29.9%), the weight of 1 gram-molecular of both proteins (C44189H71252N12428O14007S321) and glucose (C6H12O6) is jointly calculated.

The number of common atoms between two molecules namely: C, H, and O are: 44195, 71264, and 14013 respectively [17, 18, 19].

The weight of 1 gram-molecular of both protein (C44189H71252N12428O14007S321) and glucose (C6H12O6) \rightarrow 532864.58 (C) + 71834.112 (H) + 224193.99 (O) + 174079 (N) + 10291.26 (S) = 1013262.9 g

ii) The weight of protein and glucose existing in this liver tissue is:

 $\frac{29.9}{100} \times 2000 = 598 \text{ g} \text{ (Protein and Glucose)}$

iii) The weight of existent carbon in glycogen is: $\frac{532864.58}{1013262.9} \times 598 = 315.116 \text{ g (C)}$ iv) Similarly, the weight of existent hydrogen, oxygen, nitrogen, and sulphur are also calculated as below:

For hydrogen:
$$\frac{71834.112}{1011224.5} \times 598 = 42.479 \text{ g (H)}$$

For oxygen:
$$\frac{224193.99}{1011224.5} \times 598 = 132.579 \text{ g (O)}$$

For nitrogen:
$$\frac{174079}{1011224.5} \times 598 = 102.943$$
 g (N)

For sulphur:
$$\frac{10291.26}{1011224.5} \times 598 = 6.085 \text{ g (S)}$$

(IV)

i) Therefore, the total mass of each element existing in the mentioned tissue is shown below:

For hydrogen \rightarrow 155.975 g + 0.444 g + 42.479 g = 198.898 g (H)

For oxygen \rightarrow 1237.824 g + 3.528 g + 132.579 g = 1373.931 g (O)

For carbon \rightarrow 3.027 g + 315.116 g = 318.143 g (C)

For nitrogen \rightarrow 102.943 g (N)

For sulphur \rightarrow 6.085 g (S)

ii) In this state, the amounts of H and O are incorporated into the water:

 $1 \text{ H2O} = 2\text{H} + \text{O} \rightarrow \text{the amount of water because}$ incorporating the hydrogen and oxygen will be: 85.876 g (H2O)

In this stage, the obtained results are defined for the MCNP code, and are inputted to this code. On the other hand, decomposed tissue gets virtually irradiated by neutron beam, and the results are specified for a wide range of energies [20, 21].

Since the related simulation is associated with the MCNP code and it is required a big data to be illustrated, to better illustrate the simulation and its results, a part of the results extracted from the MCNP code are shown as follows.

cell 1		
energy		
1.0000E-09	1.94921E-15	0.3250
5.0000E-09	3.80572E-14	0.1701
1.0000E-08	8.80861E-14	0.1604
2.0000E-08	4.70396E-13	0.1160
4.0000E-08	1.93888E-12	0.1025
6.0000E-08	2.24895E-12	0.0961
8.0000E-08	1.95131E-12	0.1009
1.0000E-07	1.37609E-12	0.1121
2.0000E-07	4.15864E-12	0.0975
4.0000E-07	4.19963E-12	0.0974
6.0000E-07	4.08000E-12	0.1115
8.0000E-07	3.29187E-12	0.1765
1.0000E-06	3.39642E-12	0.1548
2.0000E-06	1.84449E-11	0.0840
4.0000E-06	3.72748E-11	0.0868
6.0000E-06	4.31495E-11	0.0997
8.0000E-06	4.47444E-11	0.1083
1.0000E-05	3.98960E-11	0.1386
2.0000E-05	2.53776E-10	0.0729
4.0000E-05	5.99254E-10	0.0726
6.0000E-05	6.50503E-10	0.0786
8.0000E-05	6.32612E-10	0.0911
1.0000E-04	6.91277E-10	0.1013
2.0000E-04	3.82162E-09	0.0626
4.0000E-04	8.93638E-09	0.0593

Fig 1. A part of the results extracted from the simulation of the research by MCNP code of absorbed dose in the water of the tissue plotted by MCNP code

As shown, in the first column of the results extracted from the MCNP code, the energy groups of neutron, and the correlated absorbed doses, and the errors, respectively are illustrated.

3 Results and Discussion

As explained in the article, at first, a liver tissue was decomposed to its constituent materials, and then was simulated by the MCNP nuclear code, and was virtually irradiated by neutrons. The function of the MCNP code is that it applies MONTE-CARLO method to generate random number, and simulating a sample space, and using random processes. After many computational mathematics based on the transport equation, a population of particles like neutrons are collided, and then, the amounts of absorbed doses are obtained. The transport equation is as follows.

$$\begin{split} \Omega.\nabla\varphi(r,E,\Omega) + \mu(r,E)\varphi(r,E,\Omega) &= \\ \int_0^\infty dE' \int_{4\pi} d\Omega' \mu(r,E' \to E,\Omega' \to \Omega)\varphi(r,E',\Omega') + S(r,E,\Omega) \end{split}$$
(1)

The type and values of elements existing in the mentioned tissue are according to Table 1.

The existing elements (in the tissue)	The obtained value (g)	Percentage of the element (%)
sulphur	6.085	0.3
Carbon	318.143	15.9
Hydrogen	198.898	9.95
Oxygen	1373.931	68.7
Nitrogen	102.943	5.15
Total	2000	100

Table 1. The type and values of elements existing in the tissue

The amounts of absorbed dose are extracted by MCNP code, and illustrated in Figures 2 and 3:

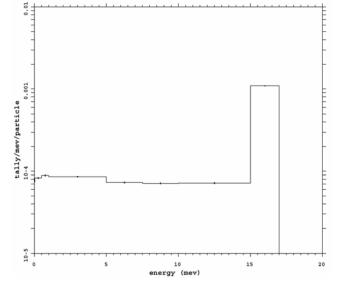


Fig 2. The amounts of absorbed dose in the water of the tissue plotted by MCNP code

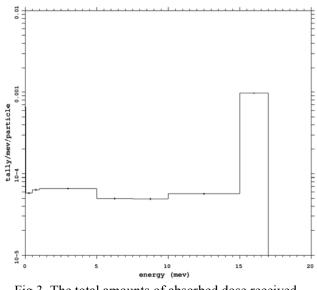


Fig 3. The total amounts of absorbed dose received by the tissue plotted by MCNP code

According to Figs. 2 and 3, the amounts of absorbed doses in water, and also the total absorbed doses are linearly changed within the neutron energy range 0-17 MeV, but there appears a sharp rise within the energy range 15-17 MeV.

4 Conclusion

As observed in Figs. 2 and 3 (extracted from the MCNP code), it can be inferred that by increasing the incident neutron energy within the fast to thermal neutron range, water receives large amounts of absorbed dose.

The current research can be generalized for other tissues like stomach and intestine.

In the ICRP report, for a wide range of energy, the conversion coefficients of fluence to effective dose have been derived from the obtained organ dose, thereby the radiation weighting factor (WR) and the tissue weighting factor (WT) are very important parameters to be considered. For instance, the skin equivalent dose conversion coefficients have been obtained for electrons and alpha particles in a parallel beam on a tissue. The high LET includes protons resulting from the capture reaction of a neutron with nitrogen, and recoil protons resulting from the collision of fast neutrons with hydrogen. The low LET of gamma rays is resulting from the capture of thermal neutrons with normal tissue and also hydrogen atoms $[1H(n,\gamma)2H]$. In addition, the high LET of protons is produced by fast neutrons scattering and also from the capture of thermal neutrons by nitrogen atoms [14N(n,p)14C].

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Contribution of individual authors to the creation of a scientific article (ghostwriting policy)

Seyed Alireza Mousavi Shirazi has carried out all of the scientific works belonging to this research consisting of calculations, simulation, and extraction of the results. In addition, he has authored and organized the paper.

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