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Energy Loss and Range Calculations for Alpha Particles in B-100 Bone and C-552 Air-Equivalent Plastic Materials

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Abstract: The type of radiation that harms humans and living organisms is the ionizing type. In this type of radiation, radiation passing through the cell transfers energy to biological tissues and causes harmful biological effects along with chemical changes. Therefore, radiation exposure doses should be kept as low as possible and appropriate shielding materials should be used between radiation and living tissue. In this study, stopping power and range calculations of B-100 bone and C-552 air-equivalent plastic materials, which are International Commission on Radiation Units & Measurement (ICRU) materials, were performed for alpha particles in the energy range of 0.1 MeV - 10 MeV. The effective charge approach within the scope of Bethe-Bloch theory and Bohr stripping criterion was used in collision stopping power calculations. The Continuous Slowing-Down Approximation (CSDA) method and the 3/8 Simpson approximation were chosen for range calculations. The error rates were found to be less than 10% when the results were compared with the available literature data.

Key words: Stopping power, CSDA range, Radiation, Alpha particles, Phantom

1. Introduction

Radiation can be divided into two groups: ionizing and non-ionizing. The type of radiation that harms humans and living organisms is the ionizing type. Ionizing radiation has cumulative effects on living organisms, especially humans, throughout their lives and increases the risk of developing cancer. In this type of radiation, radiation passing through the cell transfers energy to biological tissues and causes harmful biological effects along with chemical changes. Therefore, doses to be exposed to radiation should be kept as low as possible and appropriate shielding materials should be used between radiation and living tissue. In this respect, the energy loss (stopping power) per path taken by the charged particles in the target and the path they take (range) are significant in the interaction of radiation with matter [1].

In radiotherapy, dose accumulation and the interaction of radiation with target tissues must be understood before the patient is exposed to radiation. These interactions and dose accumulations can be investigated using phantom materials equivalent to the target of interest. Therefore, the study presented here is aimed at examining the interaction of radiation with bones and air. Although some studies have been carried out on bone and air-equivalent plastic materials so far, stopping power and range calculations of these targets have not been made for alpha particles other than ICRU [2] and the Stopping and Range of Ions in Matter (SRIM) [3].

SRIM is a group of programs that quantum mechanically describes atom and ion collisions and can perform stopping power, range and straggling calculations up to 2 GeV energy. These calculations use a statistical algorithm that consider bulk electronic excitations and bond structures between atoms. The ICRU 49 report contains tables of electronic, nuclear and total stopping power, CSDA range and deflection factors for 73 target materials for protons and alpha particles with energies between 1 keV and 1 GeV. Collision stopping powers at low energies (about 0.5 MeV for protons and below 2 MeV for alpha particles) are based on experimental data, while at energies higher than these energies they are based on Bethe stopping power theory, including quasi-empirical average excitation energies, shell corrections and the 1st Born approximation. SRIM program and ICRU report data are internationally valid and globally accepted reference databases on the interaction of radiation with matter.

In this study, stopping power and range calculations were made analytically for B-100 bone and C-552 air-equivalent plastic materials, which are ICRU materials, for alpha particles in the 0.1 MeV-10 MeV energy range. Effective charge approach within the scope of Bethe-Bloch theory and Bohr stripping criterion was used in collision stopping power calculations. Sapporo QZP functions [4] from Gaussian basis sets were preferred for the electronic potential energy functions of the targets. The CSDA method and the 3/8 Simpson approximation were chosen for range calculations. When the results obtained were compared with the available literature data, it was determined that the error rates were less than 10%. Therefore, stopping power and CSDA range calculations were performed with an innovative approach by using a new electronic potential energy function, taking into account the effective charge, stripping distance and effective average excitation energy of these targets.

2. Material and Method

2.1. Target materials

The materials selected in this study were B-100 bone-equivalent plastic (ICRU card 112) and C-552 air-equivalent plastic (ICRU card 116) targets, which are generally used in radiotherapy and are ICRU materials. The atomic number fraction by weight, average excitation energies (I), and densities (ρ) of the materials are given in Table 1.

Table 1. Density, composition, and mean excitation energy of B-100 and C-552 materials

Materials	Atomic number fraction by weight							I	ρ
	H	C	N	O	F	Si	Ca	(eV)	(g/cm^3)
B-100*	0.065	0.536	0.021	0.032	0.167		0.176	85.971	1.452
C-552*	0.024	0.501		0.004	0.465	0.003		86.863	1.765

* ICRU 49

2.2. Stopping power calculations

In this study, collision stopping power and CSDA range calculations were made for alpha particles in the energy range of 0.1 MeV-10 MeV in bone and water equivalent materials. As it is known, stopping power calculations of heavy charged particles consist of collision and nuclear parts. However, the contribution from the nuclear stopping power calculation to the total stopping power is negligible in the energy range of interest. Therefore, only the contributions from collision stopping power were considered here.

Collision stopping power calculations were performed within the framework of the effective charge approach [5], which includes the first Born approximation and takes into account the Bethe-Bloch theory [6]. Accordingly, the energy loss per unit length when alpha particles with velocity υ arrive at the target is given by

$$S_{coll}(\upsilon) = \frac{4\pi e^4}{m_e c^2 \beta^2} Z_1^2 Z_2^* ln\left(\frac{q_{max}}{q_{min}}\right) \tag{1}$$

Where, e is the elementary charge, m_e is the mass of the electron, c is the speed of light, $\beta = \upsilon/c$, Z_2^* is the effective charge of the target, q_{max} and q_{min} are momentum transfers. The effective charge and momentum transfers of the target can be found from the following relation:

$$Z_2^* = \int_{r_s}^{\infty} 4\pi r^2 \rho(r) dr \tag{2}$$

$$q_{max} = \frac{2m_e \upsilon}{\hbar}, \qquad q_{min} = \frac{2I^*}{\hbar\upsilon} \tag{3}$$

Here $\rho(r)$ is the electron density of the target material, r is the distance from the nucleus, r_s is the stripping distance, and I^* is the effective mean excitation energy of target material.

$$lnI^* = \frac{1}{Z_2^*} \int_{r_s}^{\infty} ln\left[\gamma\hbar\omega_p(r)\right] 4\pi r^2 \rho(r) dr \tag{4}$$

ω_p is the plasma frequency, and γ is the a constant that can be set to $\sqrt{2}$. The electronic potential energy function

$$U(r_s) = [-\pi\rho(r) r^4]/5 + C \tag{5}$$

obtained from the solution of Poisson's equation and the Bohr stripping criterion [7] expression were used [8]. and C is a constant. In this study, the charge density of the target materials was calculated using the expression

$$\rho(r) = \sum_{\mu} \left|u_{\mu}(\mathbf{r})\right|^2 \tag{6}$$

2.3. Gaussian basis sets

Sapporo QZP functions [9] from Gaussian basis sets were preferred to calculate the electronic charge density. This function, which consists of radial and angular parts, is as follows:

$$g(r,\theta,\phi) = N(l,\alpha) r^l e^{-\alpha r^2} Y_{l,m}(\theta,\phi) \tag{7}$$

Where l is angular momentum quantum number, $Y_{l,m}$, is spherical harmonics, α, is exponential coefficient, and $N(l,\alpha)$ is the normalization constant and is given as follows:

$$N(l,\alpha) = \frac{2\left(2\alpha_{n,l}\right)^{3/4}}{\pi^{1/4}} \sqrt{\frac{2^l}{(2l+1)!!}} (2\alpha_{n,l})^l \tag{8}$$

Here, atomic orbitals are considered to be spherical ($l = 0$) and spin interactions are ignored.

2.4. CSDA range calculations

The range calculations of alpha particles were based on the continuous slowing down approximation (CSDA), which describes the path taken by these particles as they lose energy until they continuously slow down and run out of energy:

$$R = \rho_t \int_{E_i}^{E_f} \frac{dE}{S_{coll}} \tag{9}$$

Here ρ_t is the density of the target, E_i and E_f are the initial and final energies of the alpha particles, respectively. Since this integral is very difficult to calculate analytically for range calculations, the more convenient Simpson 3/8 method, known as the four-point approximation, was used:

$$\int_{E_i}^{E_f} \frac{dE}{S_{coll}} \cong \frac{3}{8}\Delta E \left[\frac{1}{S_{coll}}(E_i) + \frac{1}{S_{coll}}(E_f) + 3\sum_{\substack{j=1 \\ 1,2,4,5}}^{n-1} \frac{1}{S_{coll}}(E_i + j.\Delta E) + 2\sum_{\substack{j=3 \\ 3,6,9}}^{n-3} \frac{1}{S_{coll}}(E_i + j.\Delta E) \right] \tag{10}$$

3. Results and Discussion

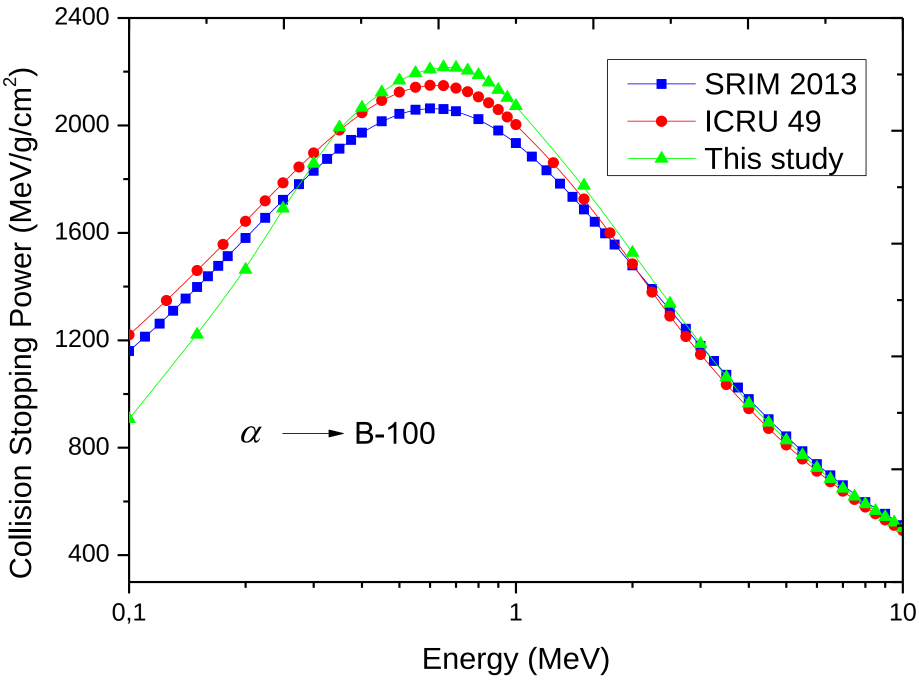

Figure 1. The collision stopping power results of B-100 bone-equivalent plastic material for alpha particles

Figure 1 shows the collision stopping power results of B-100 bone-equivalent plastic material for alpha particles with 0.1-10 MeV energy. It is understood that the values approach each other at energies of 2 MeV and above, but there are significant differences at energies lower than 2 MeV. It is particularly noteworthy that the calculated values suddenly decrease at low energies. The peaks of the curves are localized in the 600-700 keV interval, and the peak values obtained here differ from the available data. The error rates of the calculated stopping power values with the ICRU data are 2.25% in the 2-10 MeV energy range and 2.74% in the 0.1-2 MeV energy range.

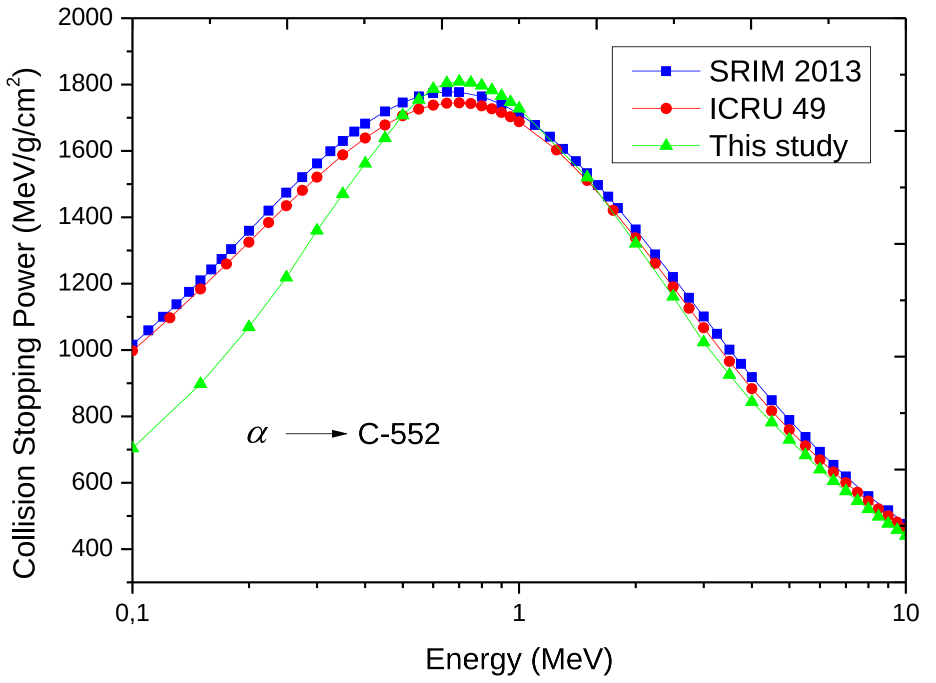

Figure 2. The collision stopping power values of the C-552 air equivalent plastic material for alpha particles

Figure 2 indicates the collision stopping power values of the C-552 air-equivalent plastic material for alpha particles in the energy range from 0.1 MeV to 10 MeV. At energies of about 1.5 MeV and above, the values are close to each other, but at energies lower than 1.5 MeV there are differences in the data. In particular, the stopping power values obtained in this study differ significantly from the existing values. The values are localized in the range of 650 keV-700 keV, with the peaks of the data being at 650 keV for SRIM and 700 keV for ICRU and this study. The error rates of the collision stopping power values calculated here with the ICRU data are 3.48% for alphas with 2-10 MeV energies and 4.08% for alphas with 0.1-2 MeV energies.

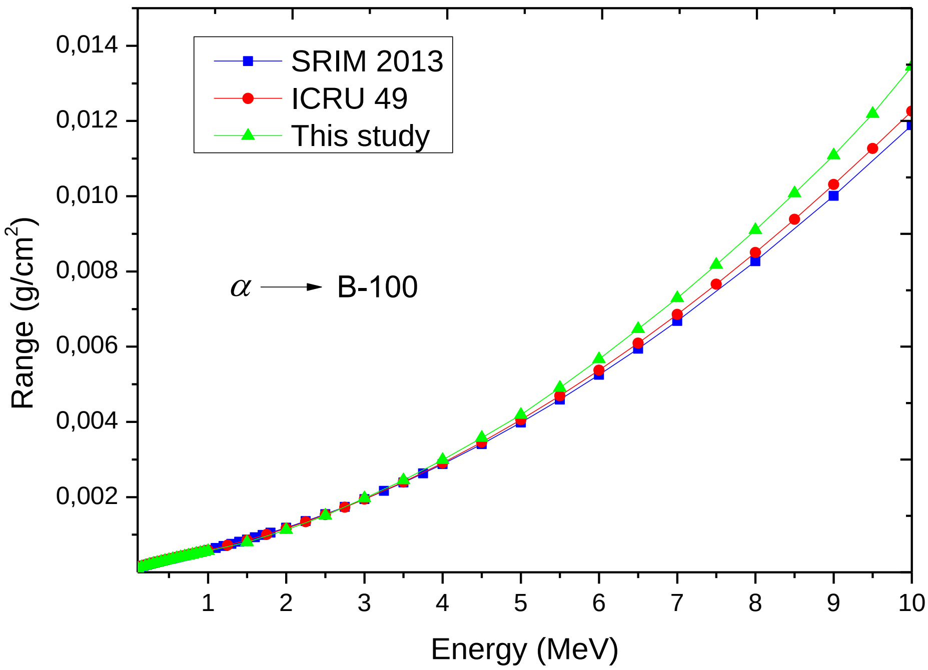

Figure 3. The CSDA range of alpha particles in B-100 bone-equivalent plastic material.

Figure 3 represents the CSDA range of alpha particles with energies of 0.1-10 MeV in B-100 bone-equivalent plastic material. The figure displays that the range values increase with the energy of the alpha particles. The envelope of the curves generally depicts the shape of a parabola. Although the SRIM values are quite close to the ICRU data, there are significant differences in the values obtained in this study. These differences become more noticeable with increasing energies, especially from 4 MeV onwards. The error rates of the CSDA range values calculated in this study with the ICRU data are 5.40% in the 0.1-2 MeV energy range, while they are at 5.14% in the 2-10 MeV energy range.

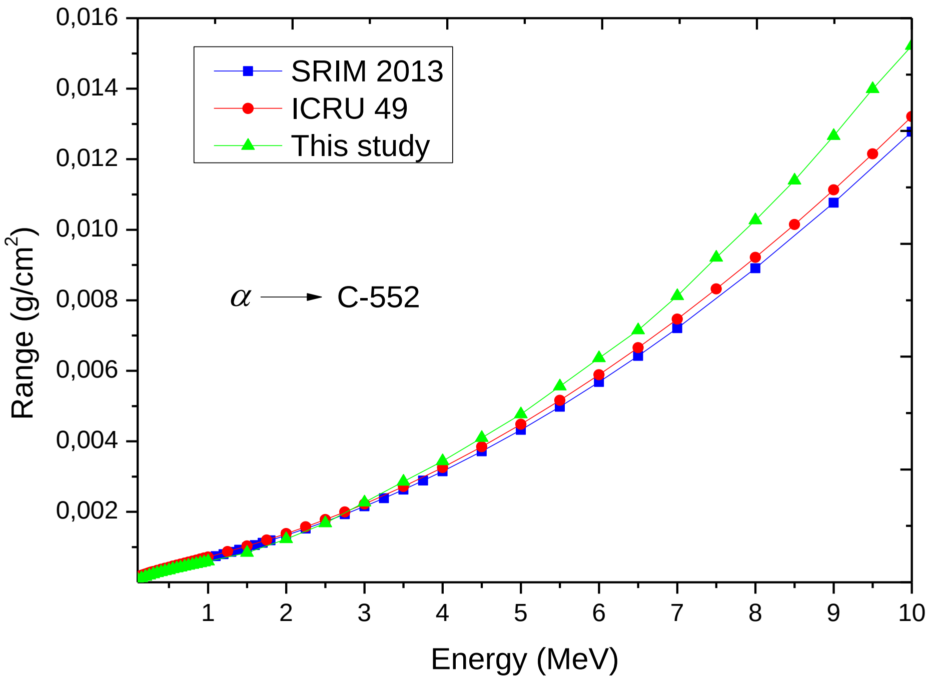

Figure 4. The CSDA range of alpha particles in C-552 air-equivalent plastic material.

Figure 4 demonstrates the CSDA range values in the C-552 air-equivalent plastic target of alpha particles with energies of 0.1-10 MeV. As expected, the range values increase proportionally with the energy of the incoming alpha particles. The amount of increase is non-linear and more in line with a parabolic curve. Again, SRIM values and ICRU data are close to each other, and the values calculated here show significant changes. The error rates of the calculated CSDA range values with the ICRU data are 6.12% in the 0.1-2 MeV range, while they are around 5.86% in the 2-10 MeV range.

In this study, collision stopping power and, indirectly, range calculations were performed using the effective charge approach within the Bethe-Bloch framework. In this approach, the 1st Born approximation is used for high-speed charged particles. So, the speeds of the incoming charged particles are greater than the orbital speeds of the electrons in the target atom. Thus, the Bohr stripping criterion and the potential energy function including the electronic charge density of the target were used to calculate the excitation cross section.

CSDA range calculations were based on the 3/8 Simpson rule. This rule approximates the function of interest, the inverse stopping power function, by a parabola, hence a 3rd-order polynomial. This further reduces the probability of error. Error rates of 5-6% in range calculations are due to the use of higher-order polynomials to connect the points and thus more accurate integral calculations. Although this method gives more accurate results than the Trapezoidal method, it would be useful to apply different integration methods such as Gaussian quadrature and Romberg method to the calculations and compare the results.

So far, many studies have been conducted using the effective charge approximation [5, 8, 10-14]. In these studies, parameters such as the atomic charge, average excitation energy, and stripping distance of different target materials were used at their effective values. In the present study, a new electronic potential energy function with the effective values of the target materials of interest was constructed and calculations based on these functions were performed. Therefore, due to these effective parameters, this method outperforms the SRIM data at energies above 2 MeV because it does not require Bloch, Barkas and shell corrections. However, the high error rates at energies lower than 2 MeV are due to the fact that the 1st Born approximation is not valid at low energies. Because additional events such as electron capture occur at these energy levels. In this region, the distorted wave Born approximation or the Coulomb wave Born approximation should be used instead of the plane wave Born approximation.

4. Conclusion

In this work, collision stopping power and CSDA range data of bone and air-equivalent plastic materials were calculated for alpha particles. Both stopping power and range values were found to be more consistent with literature data at energies above 2 MeV. In general, when averaged, it was observed that the values obtained were compatible with the ICRU data with an error rate of less than 10%. These predicted values based on the study showed good agreement with the stopping power and range values of alpha particle in SRIM code and ICRU. The data calculated in this study will provide important contributions to studies involving the interaction of radiation with matter.

Authorship contribution statement

M. Usta: Data Curation, Original Draft Writing, Visualization.

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.

Ethics Committee Approval and/or Informed Consent Information

As the authors of this study, we declare that we do not have any ethics committee approval and/or informed consent statement.

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