

Calculation of Mass Stopping Power of Alpha Particles in Human DNA Molecules Using Bragg's Rule against SRIM Simulation

Hawraa K. Ayyed*, Zahraa A. Rasheed

Department of Physics, College of Education, Al-Iraqia University, Baghdad, IRAQ
*Corresponding Author email: hawraa.k.ayyed@aliraqi.edu.iq

Abstract

The mass stopping power in different elements, molecules, and human tissues has been a subject of theoretical and applied sciences. They are very interested in mass stopping power because it characterizes how much energy a particle will lose as it passes through matter. In this paper, the mass stopping power for an alpha particle passing through DNA was calculated from 1 to 100 MeV using Bragg's rule; these results matched closely with the SRIM-2015 simulation. The mass stopping powers of the elements making up the DNA were then calculated using the Bethe-Bohr formula, and the hydrogen element has the highest stopping power among all its elements. Absorbed dose and the linear energy transfer (LET) were also calculated for DNA molecule. This work improves our understanding of how radiation deposits energy in genetic materials and helps support the use of these concepts in medical physics and assessing radiation risk.

Keywords: Mass stopping power; Bragg's rule; Alpha particles; DNA molecules

Received: April 2026; **Revised:** May 2026; **Accepted:** May 2026; **Published:** July 2026

1. Introduction

The interaction between charged particles (i.e., alpha particles, protons, electrons) and various media has been extensively researched to determine energy loss mechanisms as they pass through different materials. As a heavy charged particle travels through a medium, the predominant mechanism of energy loss is through ionization and atomic excitation of the atoms in the medium. The development of theoretical models to describe the energy losses of charged particles continues to evolve through both theoretical and experimental work; empirical and semi-empirical models of charged particle energy losses have been developed, which further the understanding of these processes and their potential applications [1,2]. In their research on energy losses of ions within solids, Bohr, Bethe, and Bloch developed theories to elucidate their energy loss. The theories' use along with a variety of empirical or semi-empirical models has provided many insights into ion energy loss due to a number of experiments performed on different target materials [3]. Stopping power of organic materials is especially important for radiation physics and biological applications; therefore, to determine total stopping power for any charged particle, you must include both collisional and radiative components to calculate how to quantify the energy released through travel through any given distance. Erosion from inelastic collision is the basic rate per unit distance that defines energy loss per travelled distance through a given vector. The ability of a charged particle to prevent itself from ionizing or exciting an electron in the material it interacts with, and the loss to bremsstrahlung radiation caused by the charged particle passing through the medium are measurable quantities called "stopping power". Stopping power is an essential characteristic to quantitatively characterize the numerous ways in which ionizing radiation interacts with different target materials and various energy levels. Stopping power, energy loss, range, absorbed dose, and straggling are all important quantities in a wide range of applications and research fields, including radiation dosimetry, medical physics, health physics, radiotherapy, nuclear physics, and radiation chemistry. The stopping power for charged particle interactions with materials is assessed using a Coulombic model to describe the interactions between the interacting charged particle and the target material. Stopping power is based on both the type of charged particle or projectile, and the type and composition of the target material [4,5]. When large particles pass through a material that absorbs their energy at an accelerating rate, the greater the loss of energy of a particle, the more times greater will be its likelihood to produce ionization events along its path as several ionization events per unit of distance, this is because the intensity of ionization ability increases as a function of the ion's velocity squared $\sim u^2$ (hence the term large particle because particle size does not affect ionization

characteristics). As a large particle spends its energy, the number of ionization events generated by that particle rises until the maximum ionization activity of the ion occurs the Bragg peak. At that time, the large particle will have lost almost absolutely all of its remaining kinetic energy [6]. The Bragg peak is representative of how a "stopping power" is affected by the thickness of the absorbing material [7].

A software application was created to store many of these analytical types of calculations and there are several software programs that do just that SRIM (Stopping Range of Ions in Matter) is an example of an application that allows the rapid calculation of ion stopping in the target material (ion range in target material, sputtering, transmission of ions, implantation of ions and to use ions in therapy) within the material being irradiated with ions [8]. In addition, SRIM can also provide data on stopping powers, expected (predicted) range for the ions and distribution for a single ion over a large number of energies through the use of elemental targets [9]. This study aims to calculate the mass stopping power of α -particles within a human DNA molecule inside living tissue within an energy range of (1–100) MeV in order to understand the mechanism of energy loss and deposition at the molecular level in biological systems.

2. Theory

2.1 DNA structure

Deoxyribonucleic acid (DNA) is an organic molecule characterized by a distinct molecular structure present in all prokaryotic and eukaryotic organisms. It is a collection of molecules that facilitate the transfer and transmission of genetic material or instructions from progenitors to their descendants. The DNA structure dictates the fundamental genetic composition of human bodies and, in fact, governs the genetic composition of nearly all life forms on Earth [10]. As shown in Fig. (1), DNA is a polymeric molecule. known building blocks stranded-It consists of repeating single as nucleotides, each nucleotide consisting of [11,12]:

- 1- Pentose sugar (deoxyribose), its molecular formula is $C_5H_{10}O_4$.
- 2- Phosphate group (Phosphateion PO_4^{-3}) consists of a central Phosphorus atom surrounded by four oxygen atoms, linked to the hydroxyl group on Carbon atom 5' of the deoxyribose sugar.
- 3- Four types of Nitrogenous bases.
 - Adenine (A) $C_5H_5N_5$
 - Guanine (G) $C_5H_5N_5O$
 - Cytosine (C) $C_4H_5N_3O$
 - Thymine (T) $C_5H_6N_2O_2$
- 4- Chemical bonds, including:
 - Phosphodiester bonds: Phosphate groups link deoxyribose sugars.
 - Hydrogen bonds: These bond between nitrogenous bases with three links (A-T) and three links (G-C).
 - Glycosid bonds: These link the nitrogenous base to the deoxyribose sugar.

The overall chemical formula of DNA is ($C_{459}H_{582}N_{162}O_{290}P_{46}$), it is not fixed and varies according to the length of the chain and the composition of the bases, but a single nucleotide can be represented by the general formula for an adenine nucleotide. This complex chemical structure is what enables it to store genetic information and transmit it across generations [13].

2.2 Mass stopping power calculation

The mass stopping power is calculated using the classical Bethe-Bohr formula, the most common material through method for calculating the energy loss rate of ionizing radiation as it passes, compounds, elements, etc. It is mathematically expressed as $(-dE/dx)$, where the negative sign indicates that the particle's energy decreases with distance. This formula appears in several equivalent forms in the scientific literature. The precise formulation depends on the authors' choice of defining the physical quantities involved and the criteria used in the derivation. Among the formulas derived from this general relationship is the Bethe-Bohr formula used to calculate the mass stopping power of the constituent elements of the DNA molecule (H, C, N, O, and P) which is given as follows [14,15], for alpha particles over an energy range from 1 to 100 MeV.

$$-\frac{dE}{dx} = \frac{4\pi n Z^2 K_0^2 e^4}{m_0 v^2} \left[\ln \frac{2m_0 v^2}{I} \right] \quad (1)$$

Where n is the number of electrons per unit volume in the stopping material, Z is the charge of the falling particle, m_0 is the rest mass of the electron, v is the velocity of the fallen particle, e is the electron charge, I is the average excitation energy of the medium ionization potential, and $(K_0 = \frac{1}{4\pi\epsilon_0})$

This equation shows that the stopping power depends on the charge, speed of charged particles, atomic density, and the number of electrons in the atom within the absorbing material [15]. The classical Bethe-Bohr formula does not include relativistic corrections such as shell, Barkas, and density corrections.

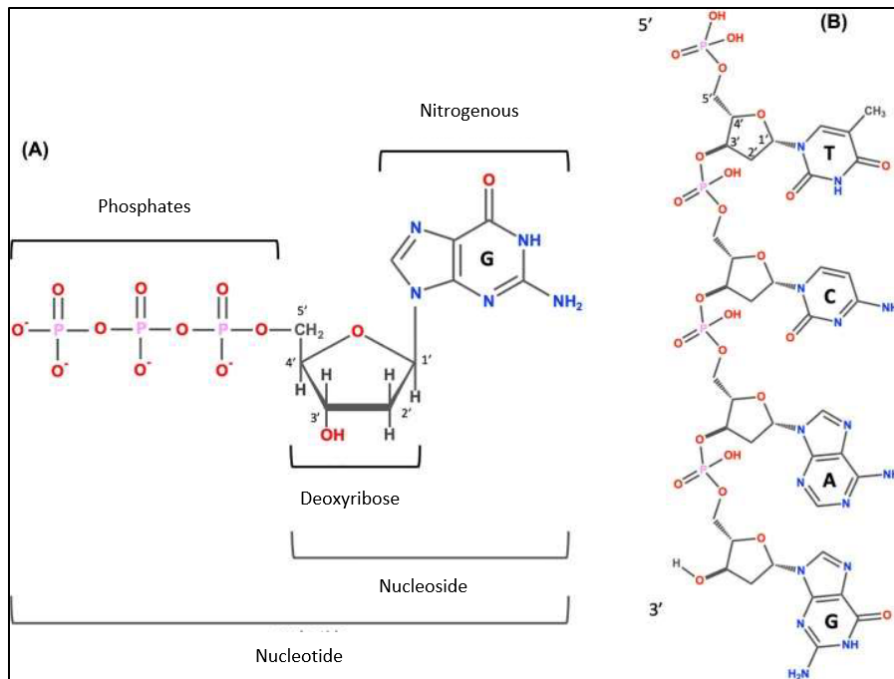


Fig. (1) The biochemical structure of DNA. (A): Nucleotide structure. (B): Part of DNA strand [10]

Bragg's rule for composite targets is commonly used to calculate the stopping power of compounds. According to this rule, the stopping power of a compound is calculated by the linear sum of the stopping powers of its individual constituent elements. In the case of a compound or molecule consisting of more than one element, to obtain energy loss in a mixture or compound, the absorbing medium can be treated by making it a thin layer of pure elements. Depending on the electron density of the elements in the absorbing medium [16], the Bragg's rule can be used to calculate the mass stopping power of a DNA molecule according to the following relationship [17].

$$\left[\frac{1}{\rho} \frac{dE}{dx} \right]_{\text{compound}} = \sum_i w_i \left(\frac{1}{\rho} \frac{dE}{dx} \right)_i \quad (2)$$

Where ρ the density of aqueous DNA equal to 1 g/cm^3 [18,19], and w_i represents the weight fraction of an element which contains N_i atoms of the i^{th} element in the DNA molecule (M), then [20]

$$w_i = \frac{a_i A_i}{A_M} \quad (3)$$

where A_i is the atomic weight of i^{th} element $A_M = \sum a_i A_i$

The second method for calculating the mass stopping power of DNA molecules using the SRIM-2015 software (Stopping and Range of Ions in Matter). The SRIM program is likely the most commonly used program for calculating the stopping power of ions in different materials. The program also utilizes both Monte Carlo software to predict the energy loss of the ions at the macro and micro levels. The SRIM software system contains all of the tools necessary to simulate the interaction of ions with different materials and to calculate the penetration and energy loss of ions in all of the various materials they can be found in. In addition to manipulating ion data in a variety of material compositions, the SRIM program provides a theoretical model for how ions strike atoms (both in terms of electronic and nuclear), using data that's based on quantum mechanical principles [21,22]. The SRIM program provides researchers with a means to study the behavior of ions through pure elements, as well as mixed materials and alloys,

by allowing researchers to vary the projectile, velocity, and material combinations used in simulations. The results which can be obtained by using our tool are derived from base laws of physics that are constantly updated with experimental data. Improvements/refinements to the calculations and scientific integrity will occur periodically to further increase both accuracy and the scientific reliability of the final result [22].

2.3 Absorbed dose

It is the energy absorbed from ionizing radiation per unit mass. The absorbed dose is measured in rad older the (traditional) unit, defined as 100 ergs/gram. As with other historical radiation unit, the rad has been replaced with its equivalent in the International System of Units (SI) the gray defined as one joule per kilogram [23]. Thus, the two units are simply related by the equation 1 Gy = 100 rad. The absorbed dose in DNA due to interaction with alpha particles was calculated using the following formula [24,25]

$$D(\text{rad}) = \frac{d\varepsilon}{dm} = \frac{E}{1\text{gram}} \frac{1.6 \times 10^{-13} \text{ J}}{1 \text{ MeV}} \frac{10^7 \text{ erg}}{1 \text{ J}} \frac{1 \text{ rad}}{100 \text{ erg/gram}} \quad (4)$$

where E (MeV) the energy of alpha particles in one gram of living tissue that contains DNA

2.4 Linear energy transfer

The linear energy transfer of charged particles in a medium is defined by the International Commission on Radiation Units and Measurements (ICRU) as the quotient of $d\varepsilon/dl$, where $d\varepsilon$ is the average energy locally imparted to the medium by a charged particle of specific energy in traversing a distance of dl [24]. LET for heavy charged particles in a way of fundamental importance in radiological physics, dosimetry and radiological biology. The power of the saver and LET are closely related to the dose and with the biological efficacy of different types of radiation, it can be calculated using the following formula [26,27].

$$\text{LET} = -\frac{dE}{dx} \times \rho \quad (5)$$

where $-\frac{dE}{dx}$ the mass stopping power for DNA molecule and ρ the density of aqueous DNA equal to 1 g/cm³

2.5 Root mean square error (RMSE)

It is a common measure for assessing the accuracy of predictive results for mass stopping power values using the following equation [28]:

$$\text{RMSE} = \sqrt{\frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2} \quad (6)$$

Where y_i the expected values of mass stopping power by using Bragg's rule values, \hat{y}_i the actual values of mass stopping power using SRIM-2015 simulation, and n represents the number of values and equals 53

3. Results and Discussion

The mass stopping power of alpha particles in interaction with DNA molecule was determined by applying Eq. 2 (Bragg's rule) and SRIM-2015 simulation program within an energy range of 1–100 MeV, table (1) shows the elemental composition of DNA molecule according to chemical formula (C₄₅₉H₅₈₂N₁₆₂O₂₉₀P₄₆). The equations were applied in the MATLAB-2016 program to produce table (2), which shows the mass stopping power of the human DNA molecule and compares the current work results with those obtained from the SRIM-2015 program.

Table (1) The chemical composition of DNA [12,29]

The element	Weight fraction
H	0.0406
C	0.3820
N	0.1572
O	0.3215
P	0.0987
Sum	1.0000

Figure (2) shows the mass stopping power of alpha particles in DNA's chemical makeup, which includes hydrogen, carbon, nitrogen, oxygen, and phosphorus. The results indicate that hydrogen contributes the most to the mass stopping power of the DNA molecule in living cells due to its higher atomic number to mass ratio compared to other elements and its low average ionization potential, making it the most effective medium in dissipating the energy of charged particles. The hydrogen atom is the most responsible for energy loss in compounds and human tissues, and contains particles in the path of alpha particle ions and has a higher probability of interacting and losing more energy, so its mass stopping power is higher than that of other elements. This result confirms the study by (Hameed 2025), which calculated the stopping power of alpha particles in the eye tissue [30].

Table (2) and figure (3) show a great overall match between the present study (using Bragg's rule to determine stopping power) and the SRIM-2015 simulation results. This shows that even though Bragg's rule is simple to use, it can be used to accurately estimate the mass stopping power of human DNA. The main goal of this study is to determine how well Bragg's rule works for finding the stopping power for a complex biological molecule like DNA. Bragg's rule is one of the more common ways to determine stopping power for compounds in that the stopping powers for compounds are determined by a weighted average of the individual elements' stopping powers. The SRIM program is much more complex than Bragg's rule in that it uses physical models and semi-empirical equations to derive a very accurate calculation of the interaction of ions with a material; the SRIM results can be used as a reference point for comparison. It has been demonstrated that the mass stopping power of alpha particles, which have a medium energy range of 1 to 100 MeV, is most effectively predicted by the Bragg rule for a particle's range in DNA, and that the main interaction of an alpha particle with the medium occurs through the excitation and ionization of atoms.

The accuracy of SRIM results in the energy range (1-100 MeV) relies on the binary collision approximation (BCA) hypothesis, which, despite its strength in describing interactions between ions and matter, overlooks the fine molecular effects of covalent bonds in DNA. The results of SRIM also remain approximate concerning environmental effects (such as the presence of water and ions surrounding the DNA). However, this range falls within the globally accepted accuracy of the program, making SRIM a reliable benchmark for comparing analytical calculations based on the Bethe-Bohr equation.

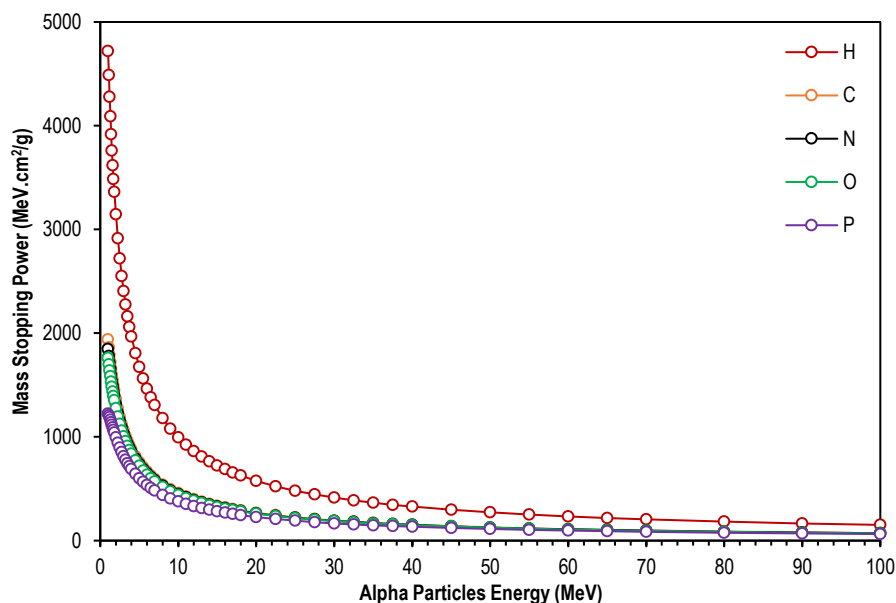


Fig. (2) The mass stopping power of DNA molecule components

At very low energies, SRIM simulations are not sufficiently accurate, especially in the field of advanced biological research. It is always preferable to rely on Geant4-DNA because it treats DNA as a real molecular structure rather than an atomic mixture, making it more accurate than SRIM in this context. It is well known that the structure of DNA consists of the double helix, base stacking, and the hydration shell, which plays a pivotal role in energy transfer. In the homogeneous model, these

components are represented by the effective density of the material, which is an acceptable approximation in the calculations of molecular stopping power for particles with energy in the studied range. However, it does not cover the local effects that occur at the nanometer level. SRIM simulation does not mimic the path structure as precise geometric modeling does, nor does it include the water layer, nor does it track the microscopic path of alpha particle interactions with electrons at each energy level, as the advanced simulation program Geant4-DNA does.

Table (2) Mass stopping power in DNA and its constituent elements over the energy range (1-100) MeV

E (MeV)	Mass Stopping power $\times 10^3$ by Bethe MeV/(g/cm ²)					Mass Stopping power MeV/(g/cm ²) for DNA molecule	
	H	C	N	O	P	Bragg's rule	SRIM-2015
1.00	4.7198	1.9405	1.8477	1.7604	1.2245	2397.4052	2399.803
1.10	4.4875	1.8631	1.7788	1.6995	1.2092	2290.7672	2293.058
1.20	4.2782	1.7908	1.7135	1.6408	1.1888	2193.0363	2193.136
1.30	4.0889	1.7234	1.6522	1.5851	1.1656	2103.4459	2105.549
1.40	3.9170	1.6608	1.5947	1.5324	1.1410	2021.1807	2023.202
1.50	3.7603	1.6027	1.5410	1.4829	1.1159	1945.5374	1947.483
1.60	3.6169	1.5486	1.4908	1.4364	1.0909	1875.7625	1877.638
1.70	3.4851	1.4983	1.4439	1.3927	1.0663	1811.2389	1811.239
1.80	3.3636	1.4514	1.4000	1.3517	1.0422	1751.4265	1751.426
2.00	3.1469	1.3665	1.3203	1.2768	0.9964	1643.9822	1645.626
2.25	2.9161	1.2745	1.2335	1.1948	0.9437	1528.5608	1530.089
2.50	2.7202	1.1952	1.1583	1.1236	0.8960	1429.8475	1431.277
2.75	2.5516	1.1262	1.0927	1.0611	0.8530	1344.3975	1345.742
3.00	2.4048	1.0655	1.0348	1.0059	0.8141	1269.6213	1269.602
3.25	2.2758	1.0117	0.9833	0.9567	0.7787	1203.6103	1204.814
3.50	2.1613	0.9636	0.9373	0.9126	0.7466	1144.8274	1145.972
3.75	2.0590	0.9204	0.8959	0.8728	0.7172	1092.1484	1093.241
4.00	1.9669	0.8814	0.8583	0.8367	0.6903	1044.6153	1045.660
4.50	1.8078	0.8134	0.7929	0.7737	0.6426	962.1842	963.146
5.00	1.6749	0.7561	0.7377	0.7204	0.6017	893.0279	893.921
5.50	1.5620	0.7072	0.6905	0.6748	0.5662	834.1302	834.964
6.00	1.4647	0.6648	0.6495	0.6351	0.5351	783.2067	783.990
6.50	1.3800	0.6278	0.6136	0.6004	0.5076	738.8051	739.544
7.00	1.3055	0.5950	0.5819	0.5696	0.4830	699.6253	700.325
8.00	1.1802	0.5397	0.5283	0.5175	0.4412	633.6161	634.250
9.00	1.0788	0.4947	0.4845	0.4750	0.4067	580.0319	580.612
10.00	0.9948	0.4573	0.4481	0.4395	0.3777	535.5482	535.548
11.00	0.9241	0.4256	0.4173	0.4095	0.3529	498.0115	498.509
12.00	0.8635	0.3985	0.3908	0.3837	0.3316	465.8315	466.297
13.00	0.8111	0.3748	0.3678	0.3612	0.3129	437.8977	438.336
14.00	0.7652	0.3541	0.3476	0.3415	0.2964	413.4372	413.851
15.00	0.7246	0.3358	0.3297	0.3240	0.2817	391.7868	392.179
16.00	0.6885	0.3194	0.3137	0.3083	0.2686	372.4755	372.848
17.00	0.6561	0.3047	0.2993	0.2943	0.2568	355.1572	355.157
18.00	0.6268	0.2914	0.2863	0.2816	0.2460	339.4873	339.487
20.00	0.5761	0.2683	0.2637	0.2594	0.2272	312.3055	312.306
22.50	0.5240	0.2445	0.2404	0.2366	0.2078	284.3512	284.351
25.00	0.4812	0.2248	0.2212	0.2178	0.1917	261.3310	261.331
27.50	0.4453	0.2084	0.2050	0.2019	0.1781	242.0215	242.021
30.00	0.4148	0.1943	0.1913	0.1884	0.1665	225.5817	225.582
32.50	0.3885	0.1822	0.1794	0.1767	0.1564	211.4010	211.401
35.00	0.3655	0.1716	0.1690	0.1665	0.1476	199.0013	199.001
37.50	0.3453	0.1622	0.1598	0.1575	0.1398	188.0753	188.263
40.00	0.3274	0.1540	0.1517	0.1495	0.1328	178.4236	178.602
45.00	0.2970	0.1398	0.1378	0.1359	0.1210	161.9527	162.115
50.00	0.2721	0.1283	0.1264	0.1247	0.1112	148.4798	148.628
55.00	0.2513	0.1186	0.1169	0.1154	0.1030	137.2127	137.350
60.00	0.2336	0.1104	0.1088	0.1074	0.0960	127.6231	127.751
65.00	0.2184	0.1033	0.1019	0.1006	0.0900	119.3897	119.509
70.00	0.2052	0.0971	0.0958	0.0946	0.0848	112.2076	112.320
80.00	0.1834	0.0869	0.0857	0.0847	0.0760	100.3497	100.570
90.00	0.1660	0.0787	0.0777	0.0768	0.0690	90.8773	90.835
100.00	0.1518	0.0721	0.0712	0.0703	0.0633	83.1642	83.144

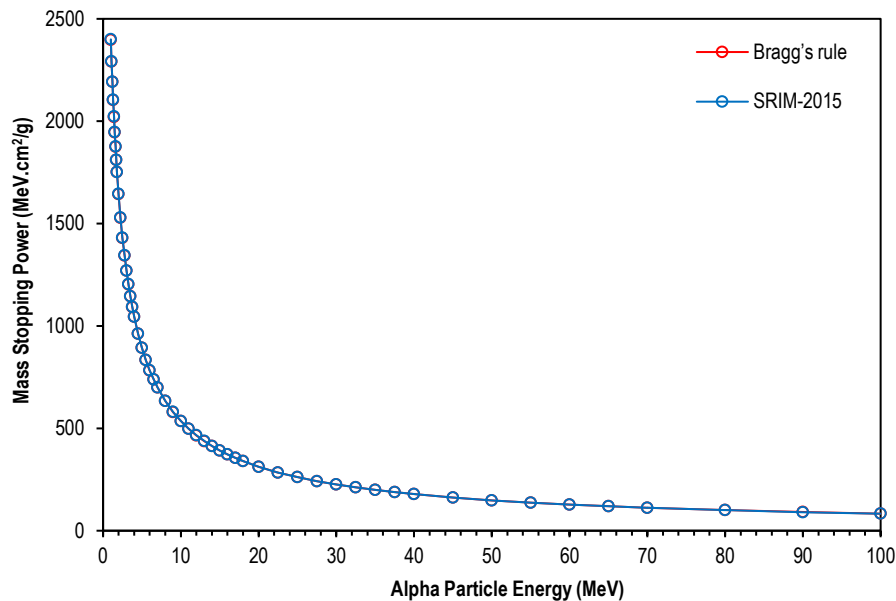


Fig. (3) Comparison of mass stopping power using the Bragg rule and SRIM-2015 program as a function of alpha particle energy

Table (3) represents the absorbed dose (D) and linear energy transfer (LET) in DNA molecule using equations (4 and 5). The absorbed dose gradually increases with the increase in energy from 1 to 100 MeV because the amount of energy deposited in the material becomes greater with higher energy, which makes sense if higher energy particles are capable of transferring more energy along the studied path. Table (3) indicates that increasing the particle energy from 1 to 100 MeV leads to a gradual decrease in LET values from 2397.4052 to 83.1642 MeV/cm. This behavior can be explained by the fact that the LET represents the amount of energy lost per unit length (MeV/cm). Therefore, when the alpha particle energy increases, its speed increases, and the duration of its interaction with the medium along the path decreases, causing the energy to be distributed over a greater distance and the energy deposition density to be lower. In other words, a high-energy particle traverses the medium in a "more dispersed" manner with lower energy deposition density compared to a low energy particle, which leaves more concentrated damage; the decrease in LET with increasing energy does not necessarily mean a decrease in the total deposited energy, but rather that the deposition has become less dense along the path. This behavior is critical in the radiological effects on DNA because higher LET values are usually associated with more severe and localized damage, such as double-strand breaks, while lower values mean more dispersed and less dense deposition. Thus, this result reflects the expected inverse relationship between particle energy and LET in this energy range.

The relative biological effectiveness (RBE) is closely and non-linearly related to LET, where the LET value is the physical standard that determines the efficiency of radiation in causing biological damage compared to a reference radiation (such as X-rays). The RBE increases with increasing LET because higher LET radiation deposits its energy more densely along its path, increasing the likelihood of causing "double-strand breaks in the DNA" (DSBs) that are difficult for the cell to repair. At the peak point (100 keV/μm), the RBE reaches its maximum value, which is considered the "ideal" value for causing lethal DNA damage by depositing energy within the microscopic distance around the DNA. The decline after the peak (Overkill Effect): Interestingly, the RBE decreases if the LET continues to increase above 100 keV/μm; this is due to the phenomenon of "overkill," where the particle deposits much more energy than the cell needs to die, resulting in a "waste" of energy without a corresponding increase in additional biological effect [24]. The main challenges in evaluating the relative biological effectiveness (RBE) of high linear energy transfer (LET) radiation in DNA are:

- Overkill Effect: High LET values lead to excessive energy deposition, resulting in biological energy waste and inaccurate RBE measurements due to assumptions of direct relationships between energy and biological effects.

- Reference Dose Determination: The variation in DNA damage types complicates establishing a biologically equivalent reference dose for comparison with traditional radiation (like X-rays) [24].
- Technical Limitations: Measuring effects at high LET requires advanced precision techniques (Nanosimetry) to understand particle interactions with DNA, as average absorbed dose simulations do not capture essential spatial biochemical reaction distributions [31].
- Cellular Repair Mechanism Interference: The clustered nature of damage at high LET disrupts regular DNA repair processes, leading to variable RBE values influenced by cell type, cycle, and repair capacity, necessitating individualized biological assessments [32].

Table (3) Absorbed dose and linear energy transfer for DNA

E (MeV)	Absorbed dose× 10 ⁻⁸ (rad)	LET (MeV/cm)
1.00	1.60	2397.4052
1.10	1.76	2290.7672
1.20	1.92	2193.0363
1.30	2.08	2103.4459
1.40	2.24	2021.1807
1.50	2.40	1945.5374
1.60	2.56	1875.7625
1.70	2.72	1811.2389
1.80	2.88	1751.4265
2.00	3.20	1643.9822
2.25	3.60	1528.5608
2.50	4.00	1429.8475
2.75	4.40	1344.3975
3.00	4.80	1269.6213
3.25	5.20	1203.6103
3.50	5.60	1144.8274
3.75	6.00	1092.1484
4.00	6.40	1044.6153
4.50	7.20	962.1842
5.00	8.00	893.0279
5.50	8.80	834.1302
6.00	9.60	783.2067
6.50	10.40	738.8051
7.00	11.20	699.6253
8.00	12.80	633.6161
9.00	14.40	580.0319
10.00	16.00	535.5482
11.00	17.60	498.0115
12.00	19.20	465.8315
13.00	20.80	437.8977
14.00	22.40	413.4372
15.00	24.00	391.7868
16.00	25.60	372.4755
17.00	27.20	355.1572
18.00	28.80	339.4873
20.00	32.00	312.3055
22.50	36.00	284.3512
25.00	40.00	261.3310
27.50	44.00	242.0215
30.00	48.00	225.5817
32.50	52.00	211.4010
35.00	56.00	199.0013
37.50	60.00	188.0753
40.00	64.00	178.4236
45.00	72.00	161.9527
50.00	80.00	148.4798
55.00	88.00	137.2127
60.00	96.00	127.6231
65.00	104.00	119.3897
70.00	112.00	112.2076
80.00	128.00	100.3497
90.00	144.00	90.8773
100.00	160.00	83.1642

The root mean square error was calculated using Equation 6. A comparison of the mass stopping power calculated using the Bragg equation with the results of the SRIM-2015 simulation program showed an RMSE = 0.94 Mev.cm²/g, reflecting excellent analytical accuracy of the approximate equation compared to the standard Monte Carlo method. This value indicates a high degree of agreement between the two methods within the studied energy range.

4. Conclusion

From this study, we conclude that hydrogen has the greatest mass stopping power of alpha particles (from all DNA components), according to the mass stopping powers calculated to be in the energy range of 1-100 MeV using Bethe-Bohr formula, followed by carbon, nitrogen, and oxygen, with phosphorus being the least efficient. Thus, the above order results from the mass stopping power's dependence on the ratio (Z , atomic number to A , the sum total of the protons and neutrons) and the average ionization energy (I) because it makes lighter elements better at providing relative stopping per unit of mass in this type of calculation. Also, when the energy of alpha particles (i.e., their velocity) increases, the time of their interaction with the electrons of the material decreases, reducing the effectiveness of energy exchange through electrostatic forces. As a result, the rate of energy loss per unit distance (i.e., stopping power) decreases, allowing the particle to penetrate to a greater depth before losing all its energy and stopping. A slow (low energy) of alpha particle dissipates more energy through ionization of atoms than a rapid (high energy) alpha particle, as the slower particle remains in an atom for an extended duration, hence increasing the likelihood of an electronic transition occurring within the atom. There is a good agreement between the mass stopping power curve obtained in the current work using the Bragg's rule and the SRIM-2015 simulated curve for a human DNA molecule as a function of alpha particle energy. The decrease in linear energy transfer (LET) values with increasing alpha particle energy results in a less dense distribution of deposited energy, reducing the concentration of DNA damage. High LET values are associated with severe damage such as double-strand breaks, while low values lead to more dispersed deposition.

References

- [1] Z.J. Raheem, "Stopping Power and range of heavy ions in human body tissues". Ph.D. thesis, University of Baghdad-Iraq (2019).
- [2] L.E. Porter, "Further Observations of Projectile-z Dependence in Target Parameters of Modified Bethe-Bloch Theory", *Int. J. Quantum Chem.*, 95 (2003) 504-511.
- [3] M.O. Ghossain, "Calculations of Stopping Power, and Range of Ions Radiation (Alpha Particles) Interaction with Different Materials and Human Body Parts", *Int. J. Phys.*, 5 (2017) 92-98.
- [4] A.A. Correa, "Calculating electronic stopping power in materials from first principles", *Comput. Mater. Sci.*, 150 (2018) 291-303.
- [5] L.A. Susam et al., "Tailoring a Behavioral Symmetry on KERMA, Mass Stopping Power and Projected Range Parameters against Heavy-Charged Particles in Zinc-Tellurite Glasses for Nuclear Applications", *Symmetry*, 15(1201) (2023) 1-12.
- [6] J. Lilley, "**Nuclear Physics: Principles and Applications**", John Wiley & Sons (2013).
- [7] I. Tolstikhina et al., "**Basic Atomic Interactions of Accelerated Heavy Ions**", in *Matter: Atomic Interactions of Heavy Ions*, Springer Series on Atomic, Optical, and Plasma Physics, vol. 98 (2018).
- [8] J.F. Ziegler, J.P. Biersack, and M.D. Ziegler, "**SRIM-The Stopping and Range of Ions in Matter**", Ion Implantation Press (2008).
- [9] J.F. Ziegler, M.D. Ziegler, and J.P. Biersack, "SRIM-The stopping and range of ions in matter", *Nucl. Instrum. Meth. B*, 268 (2010) 1818-1823.
- [10] M.A. Ahmed et al., "Structure, Functions and Clinical Significance of DNA: A Review Article", *Int. J. Health Med. Res.*, 3(7) (2024) 464-468.
- [11] A. Travers and G. Muskhelishvili, "DNA structure and function", *The FEBS J.*, 282(12) (2015) 2279-2295.
- [12] J.D. Watson and F.H.C Crick, "Molecular Structure of Nucleic Acids: A Structure for Deoxyribose Nucleic Acid", *Nature*, 171 (1953) 737-738.
- [13] A. Agten et al., "A Compositional Model to Predict the Aggregated Isotope Distribution for Average DNA and RNA Oligonucleotides", *Metabolites*, 11(6) (2021) 400.
- [14] T.A. Younis, "Calculation of the Mass Stopping Power and Range for alpha Particle in Al₂O₃", *NeuroQuantol.*, 20(10) (2022) 2906-2912.
- [15] M.O. El-Ghossain, "Calculations of Stopping Power, and Range of Ions Radiation (Alpha Particles) Interaction with Different Materials and Human Body Parts", *Int. J. Phys.*, 5(3) (2017) 92-98.
- [16] O. Ahmed, "Stopping Power and Shell Correction From Orbital Mean Excitation Energies", M.Sc. Thesis, Al-Mustansiyah University-Iraq (2001).
- [17] W.H. Bragg and R. Kleeman. "On the α particles of radium, and their loss of range in passing through various atoms and molecules", *The London Edinburgh Dublin Philos. Mag. J. Sci.*, 10(57) (1905) 318-340.
- [18] X. Lang et al., "Probing the structure of water in individual living cells", *Nature Commun.*, 15(5271) (2024) 1-12.
- [19] R. Liénard et al., "In situ observation of proton-induced DNA fragmentation in the Bragg peak: Evidence for protective role of water", *Phys. Rev. Res.*, 7 (2025) 043004.

- [20] M. Şekerci, H. Özdoğan, and A. Kaplan, "Charged Particle Penetration Distance and Mass Stopping Power Calculations on Some Nuclear Reactor Control Rod Materials", *J. Sci. Technol., Erzincan University*, 12(2) (2019) 1103-1115.
- [21] Z. Ali et al., "Advancements in primary radiation damage models and SRIM simulations: A review of radiation damage predictions", *Nucl. Eng. Technol.*, 57 (2025) 103570.
- [22] S. Mohan and S. Lakhwant, "Electronic Stopping Power of Various Organic Compounds for Proton (0.05-10MeV): A Comparative study", *Mater. Phys. Mech.*, 12 (2011) 43-57.
- [23] T.A. Younis, "Calculation of the Stopping Power and Range for alpha particles in Some Materials and Tissues", Ph.D. thesis, University of Baghdad, Iraq (2018).
- [24] International Atomic Energy Agency, "Cytogenetic analysis for radiation dose assessment: a manual". Vienna, Technical Reports Series, no. 405 (2001).
- [25] A. Alshibel and K.T. Osman, "Mass Stopping Power and Range of Alpha Particles in Biological Human Body (Water and Eye Lens Tissue)". *Open Access Libr. J.*, 11 (2024) e11081.
- [26] P.G. Rancoita and C. Leroy, "**Principles of Radiation Interaction in Matter and Detection**", 4th ed., World Scientific (Singapore, 2016).
- [27] E.L. Alpen, "High Linear Energy Transfer Radiation Effects", Ch. 14, in **Radiation Biophysics**, 2nd ed., Academic Press (1998), pp. 365-392.
- [28] T. Chai and R.R. Draxler, "Root mean square error (RMSE) or mean absolute error (MAE)? -Arguments against avoiding RMSE in the literature", *Geosci. Model Dev.*, 7 (2014) 1247-1250.
- [29] S. Minchin and J. Lodge, "Understanding biochemistry: structure and function of nucleic acids", *Essays Biochem.*, 63(4) (2019) 433-456.
- [30] T.K. Hameed, "Calculation of stopping power, range and radiation dose of alpha particles in Eye tissue", *J. Edu. Sci. Stud., Al-Iraqia University*, 1(26) (2025) 164-172.
- [31] M.C. Joiner and A.J. Kogel, "**Basic Clinical Radiobiology**", 5th ed., CRC Press (2018).
- [32] W. Ulmer, "Aspects of linear energy transfer (LET) and relative biological effectiveness (RBE) in radiation therapy with positively charged particles and the role of electron capture", *Radiat. Phys. Chem.*, 163 (2019) 26-38.
-