

Research Article

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Density functional theory to study stopping power of proton in water, lung, bladder, and intestine

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Abstract: Stopping power, range, and time of proton in water, lung, bladder, and intestinal human tissues are calculated using density functional theory and Beth's relativistic equation in range of proton energy (0.01–1,000 MeV). The experimental data extracted from SRIM-2013 program were used to proton to the same human tissues applied in the MATLAB-2021 program, and the mean ionization potential of water and the studied tissues is calculated using Gaussian 09W program. A good agreement has been found between our calculations for stopping power, range, and time of protons in the studied human body tissues and SRIM-2013 program calculations.

Keywords: density functional theory, stopping power, range, stopping time, mean ionization potential, SRIM-2013 program, human body tissues

1 Introduction

Proton beams are used in radiotherapy to treat cancers effectively. The precise dosimetry of proton radiation is dependent on a detailed information regarding proton stopping power and range values in the substance of interest [1–7]. Calculating the stopping power and range of charged particles in matter has long been a topic of study and experimentation. In radiation physics, chemistry, medicine, microdosimetry, proton treatment, and biology, simple yet precise information on the stopping power and range values for protons is commonly required.

Stopping power and range information are crucial for characterizing phantom and radiation detector materials [8]. Many scientists have investigated proton stopping power and range in various organic materials [9,10]. However, stopping power and range data encompassing tissues are uncommon; therefore, stopping power and range information of body tissues for protons are required, especially in proton treatment. The electronic stopping power, which is based on inelastic collisions with the target's electrons, contributes the most to the total stopping power for protons. Nuclear stopping power, on the other hand, contributes the least to overall stopping power and is only important at extremely low energies due to elastic Coulomb collisions with target nucleons. For example, nuclear stopping power contributes to more than 1% of overall stopping power only at energies below 20 keV for protons in water [11].

The research aims at the possibility of adopting protons in the treatment and diagnosis of some defects in human tissues by calculating the stopping power, range, and stopping time of protons in these tissues and by studying the charge distribution based on the theory of density function.

2 Theory

The best extending formula for average energies, Bohr [12]. The effective charge Z_2^* of projectiles was provided. Yarlagadda et al. and Brandt [13,14] have detailed in full the Bohr criteria of abstraction. All outer shell electrons attached to the moving ion in orbitals with velocities less than u are removed off the target, according to the criteria. The criteria should, at the very least, be relevant to the target atom, taking into consideration the symmetry between the projectile and the target. Consider the effective atomic number Z_2^* and effective mean excitation energy I^* for the target electrons, both of which are affected by the projectile's energy. The summed corrections for Z_2 should be Z_2^* and I^* at

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Table 1: Mean ionization potential of water, lung, bladder, and intestine by different basis sets

Tissue	Basis sets					
	3-21G	6-31G	6-311G	LanL2DZ	LanL2MB	SDD
Water	88.19	88.98	89.05	88.84	86.75	88.83
Lung	137.82	139.60	139.56	129.24	125.01	137.79
Bladder	138.34	140.06	140.01	129.34	125.14	137.32
Intestine	135.56	137.18	137.14	131.69	127.32	136.29

higher energies, which are nearly similar to the inner shell adjustments; nonetheless, the values of I^* differ from those of I , which are considered energy independent. The Bethe modified formula is rewritten as [15]:

$$S_e = \frac{4\pi(Z_1^*)^2 e^4 N}{mv^2} Z_2^* \ln \left(\frac{2mv^2}{I^*} \right), \quad (1)$$

in which the effective atomic number Z^* (Z stands for Z_1 and Z_2) relationship can be calculated as follows [16]:

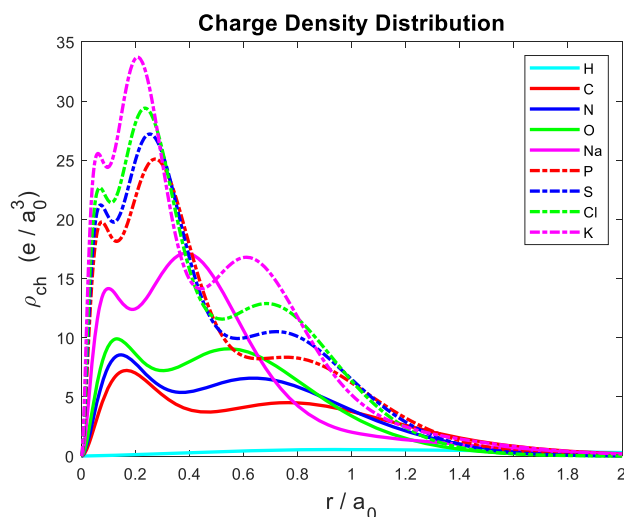
$$Z^* = 4\pi \int_{r_b}^{\infty} r^2 \rho(r) dr, \quad (2)$$

where r is the distance from the nucleus, r_b is determined from the Bohr stripping criterion $v \geq bv_F(r_b) = bh[3\pi^2 \rho(r_b)]^{1/3}$, where $v_F(r)$ is the velocity of the projectile or target atom's Thomas-Fermi orbital, b is a constant of proportional about 1.26, and $\rho(r)$ is the electronic charge density distribution in atom. The effective mean excitation energy I^* is given by the Lindhard and Scharff hypothesis [17]:

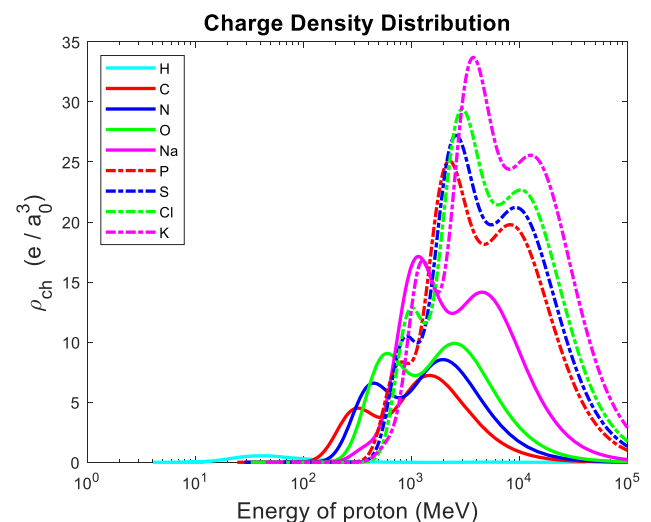
$$\ln I^* = \frac{4\pi}{Z_2^*} \int_{r_b}^{\infty} \ln[\gamma \hbar \omega_p(r)] r^2 \rho(r) dr, \quad (3)$$

Table 3: Stopping power calculations S_{total} for proton in water and studied human body tissues

Proton energy (MeV)	S_{total} (MeV cm ² /g)			
	Water	Lung	Bladder	Intestine
0.01	-9844.7612	-11141.9148	-11162.6750	-11074.2823
0.02	-2148.9928	-3056.8217	-3067.0356	-3021.4691
0.05	606.9184	106.6873	102.6895	121.6411
0.07	818.1915	424.9167	422.0841	435.8114
0.1	858.1965	556.2108	554.2450	563.9954
0.2	706.5357	529.5924	528.6260	533.6390
0.5	429.4418	344.9190	344.5410	346.6196
0.7	345.3144	281.3256	281.0579	282.5620
1	270.3860	222.9037	222.7179	223.7854
2	163.1681	136.7943	136.7029	137.2512
5	80.2856	68.3110	68.2752	68.5028
7	61.3826	52.4420	52.4165	52.5815
10	46.0344	39.4787	39.4609	39.5784
20	26.1813	22.5899	22.5810	22.6421
50	12.4774	10.8319	10.8283	10.8546
70	9.5776	8.3298	8.3271	8.3467
100	7.3013	6.3611	6.3592	6.3736
200	4.4982	3.9303	3.9292	3.9376
500	2.7463	2.4073	2.4068	2.4116
600	2.5582	2.2439	2.2433	2.2478
700	2.4285	2.1312	2.1307	2.1349
800	2.3353	2.0503	2.0499	2.0538
900	2.2664	1.9906	1.9902	1.9940
1000	2.2143	1.9456	1.9452	1.9489



(a)



(b)

Figure 1: Charge density distribution of elements in water and studied human body tissues.

where $\gamma = \sqrt{2}$ for $Z \geq 30$, and $\omega_p(r)$ is the local plasma frequency $(4\pi e^2 \rho(r)/m)^{1/2}$. A criterion was proposed by Lindhard and Scharff: $2mv^2 \geq \gamma \hbar \omega_p(r)$. However, for the time being, the Bohr stripping criteria are preferred.

Stopping power of composites and tissues is given as sum of stopping powers of its constituent elements according to the Bragg equation [18]:

$$S_{\text{com}}(E) = \sum_i w_i S_i(E), \quad (4)$$

where w_i is the weight ratio of each element in compound, and $S_i(E)$ is the stopping power in element.

The stopping range (R) is the distance traveled by the incident particle in the target material. In proton therapy, the range values are also determined as the distance between

the starting point of the target's surface and 80% of the Bragg peak. The particle range in the target material can be determined using the continuous slowing down approximation [19]:

$$R(E) = \int_E^0 -\frac{1}{S(E)} dE. \quad (5)$$

The stopping time is defined as the time required to stop the charged particle in a medium, and it can be calculated from the following integral relationship [20]:

$$t(E) = \int_E^0 -\frac{1}{vS(E)} dE, \quad (6)$$

where v is the ion velocity.

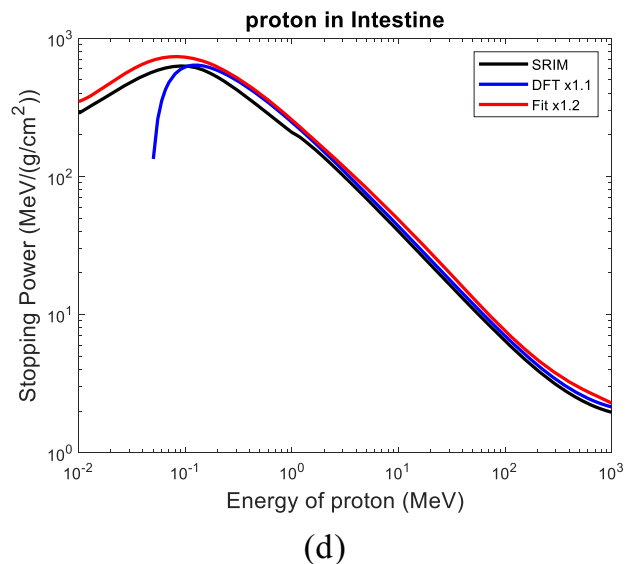
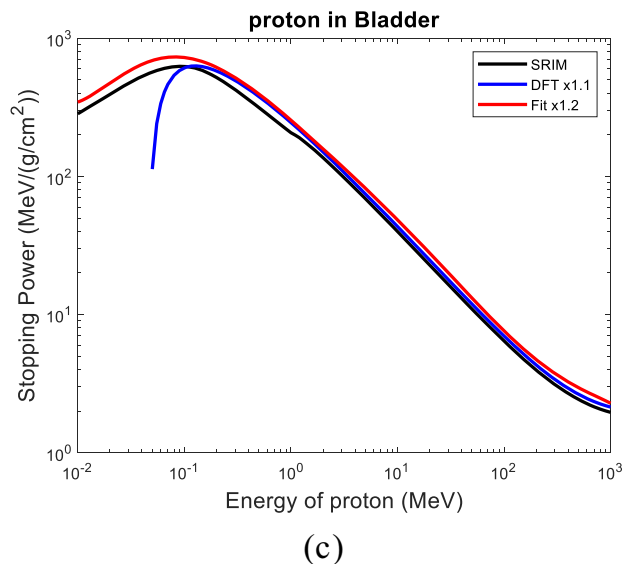
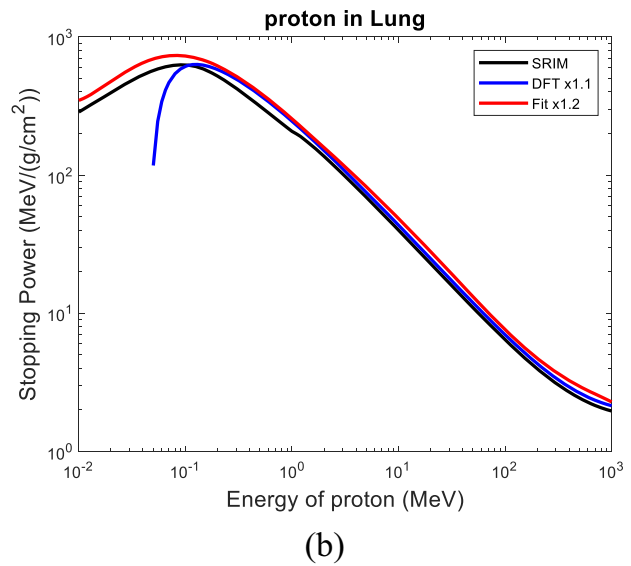
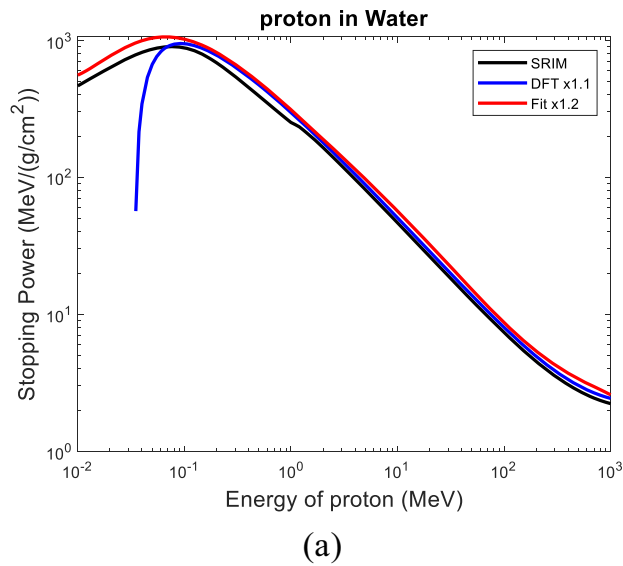


Figure 2: Stopping power calculations for proton in (a) water, (b) lung, (c) bladder, and (d) intestine.

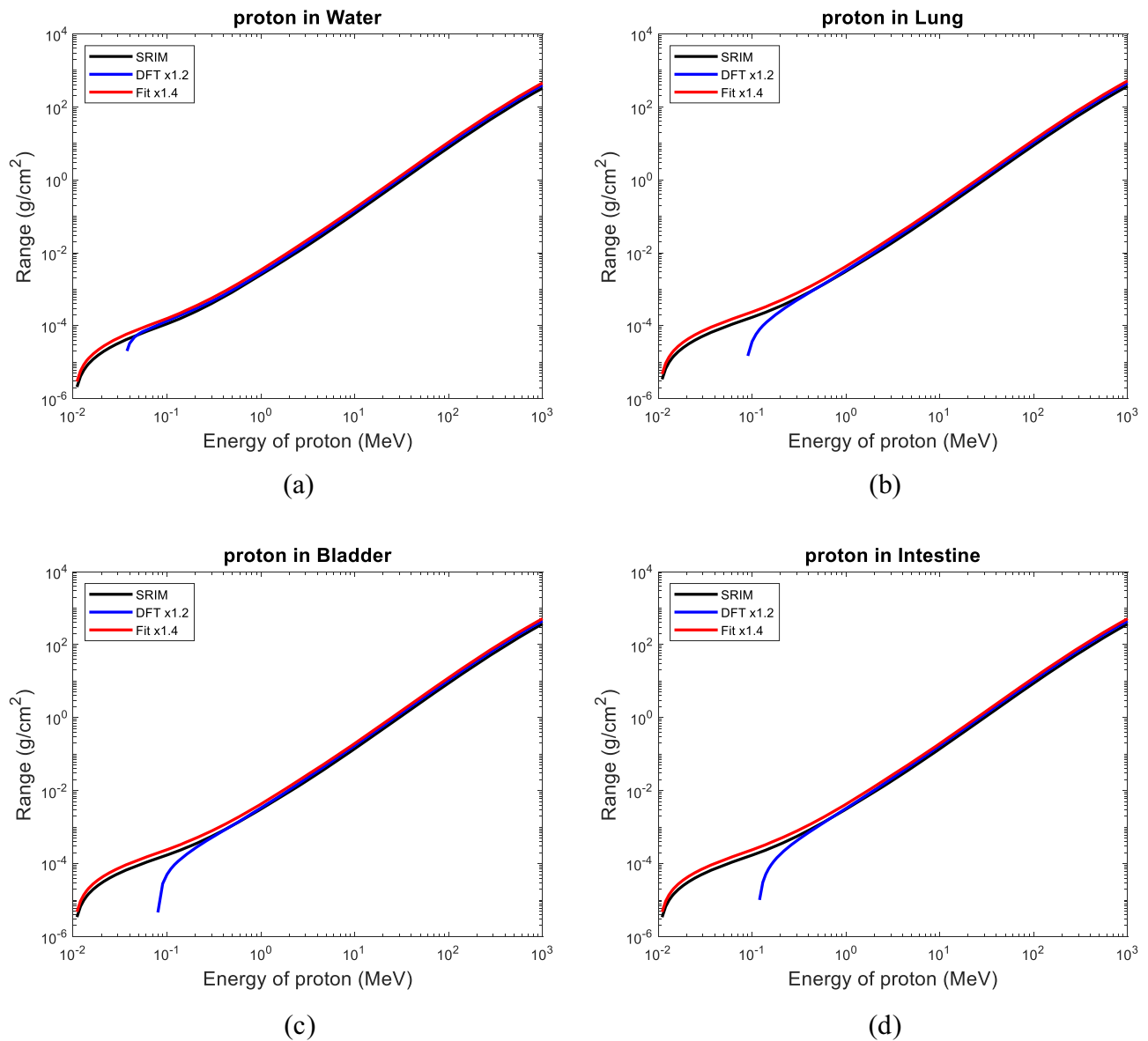


Figure 3: Range calculations of electron in (a) water, (b) lung, (c) bladder, and (d) intestine.

Table 2: Weight ratios of elements in water and studied human body tissues

Tissue	H	C	N	O	Na	P	S	Cl	K
Water	0.112	—	—	0.888	—	—	—	—	—
Lung	0.007	0.089	0.031	0.846	0.003	0.004	0.007	0.008	0.006
Bladder	0.007	0.081	0.026	0.858	0.003	0.004	0.005	0.007	0.008
Intestine	0.008	0.099	0.022	0.858	0.002	0.002	0.002	0.005	0.003

3 Results and discussion

The mean ionization potential was calculated for the constituent elements of water and studied human tissues using

Gaussian 09W program for a number of basis sets, which are 3–21G, 6–31G, 6–311G, LanL2DZ, LanL2MB, and SDD; the mean ionization potential calculations are listed in Table 1 in eV units.

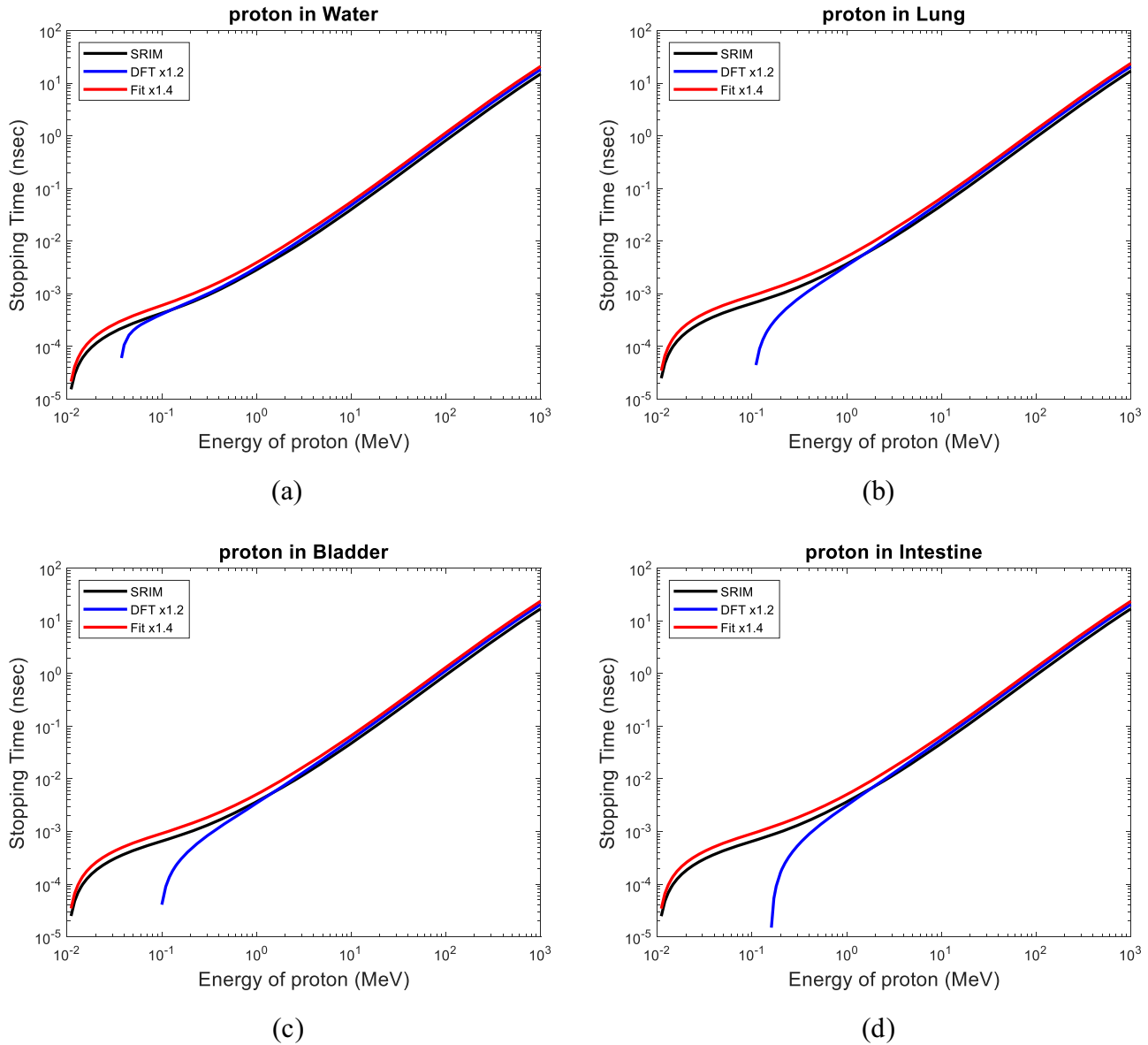


Figure 4: Stopping time calculations of electron in (a) water, (b) lung, (c) bladder, and (d) intestine.

Figure 2, Section a, shows the relationship between the charge density distribution of orbital electrons in the atoms of the elements that make up water and the studied tissues in (e/a_0) unit, and the ratio of the radial distance to the Bohr radius a_0 , while Section b shows the relationship of the electron charge density distribution with the energy of the proton. The charge density distribution curves contain several peaks representing the centers of the electronic shell in each atom, and all curves start from zero where the nucleus of the atom is, and we also note that the hydrogen atom has the lowest value for the distribution of the electronic charge density because it contains only one electron, which makes its contribution to stopping the proton. The proton in the studied human tissues is very few, while the

atoms of chlorine and potassium have the largest number of electrons among the constituent atoms, so they have the greatest values for the distribution of charge density, which makes their great contribution to stopping the proton.

The stopping power, range, and stopping time are calculated in Table 3 and Figures 1–3) using the Bethe formula and density functional theory (DFT) for water, lung, bladder, and intestine with a proton energy range from 10^{-2} to 10^3 MeV, whereas the Bethe equation (equation (1)) was used to calculate the stopping power of each of the elements that make up the water and lung, bladder, and intestine, then the stopping power for each of water and tissues was calculated from the Bragg equation (4), and the weight ratios are listed in Table 2.

The calculations of the stopping power of water, lung, bladder, and intestine are represented in Figure 2 in Sections a–d respectively, the black curve represents the calculations of the global program SRIM-2013, the blue curve represents the calculations of the relative Beth equation using the DFT, and the red curve represents the calculations of the curve-fitting formula. All calculations for the blue and red curves have been multiplied by coefficients to show the difference between the curves because they are very similar. The calculations of the stopping power are directly proportional to the energy of the projectile (proton), as it increases with the increase of energy up to the maximum value of the stopping power. Else, then, the stopping power decreases with increasing proton energy. The correlation coefficient between the practical calculations of the SRIM-2013 program and the theoretical calculations are listed in each section of Figure 1. The values of the correlation coefficient show a good agreement between the calculations of the SRIM-2013 program and the calculations of the current study, especially in the high-energy region (1–1,000 MeV).

The range and stopping time calculations calculated by equations (5) and (6) for water, lung, bladder, and intestine are represented in Figures 2 and 3 in Sections a–d, respectively, and in the same order and colors as Figure 1 for stopping power. The range and stopping time are directly proportional to the energy of proton, as they increase with the increase in energy. The correlation coefficient between the practical calculations of SRIM-2013 program and the theoretical calculations is listed at the bottom of each section of Figures 2 and 3, and they show the complete agreement between the calculations of the SRIM-2013 program and the calculations of the current study.

The ratio of the stopping range to the stopping time is directly proportional to the energy and at the same time is inversely proportional to the stopping power, which is included in the theoretical relations to calculate the range (equation (5)) and the stopping time (equation (6)).

And at the energies in which the process of ionization and irritation occurs, the effect of the denominator (stopping power) is greater than that of the numerator (energy), and at high energies, the effect of energy is clear in the results (Figure 4).

4 Conclusions

Through the research results that we reached to calculate the total stopping power using the Bethe equation by DFT

and with an energy range (0.01–1,000) MeV, it was found that the stopping power increases at low energies less than 0.1 MeV and decreases with the increase in energy greater than 0.1 MeV, where it was found through calculations that they depend on the speed projectile. By calculating the Bethe equation to calculate the total stopping power in the studies tissue, it was found that results of the curve match are close to the practical results of SRIM-2013 with approximately equal correlation coefficients $R_c = 0.9$.

Conflict of interest: Authors state no conflict of interest.

Data availability statement: The most datasets generated and/or analysed in this study are comprised in this submitted manuscript. The other datasets are available on reasonable request from the corresponding author with the attached information.

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