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Stopping power and range calculations in human tissues by using the Hartree-Fock-Roothaan wave functions

Metin Usta[a,*], Mustafa Çağatay Tufan[b]

[a] Department of Physics, Faculty of Arts and Sciences, Mustafa Kemal University, 31034 Hatay, Turkey
[b] Department of Physics, Faculty of Arts and Sciences, Ondokuz Mayıs University, 55139 Samsun, Turkey

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ABSTRACT

The object of this work is to present the consequences for the stopping power and range values of some human tissues at energies ranging from 1 MeV to 1 GeV and 1–500 MeV, respectively. The considered human tissues are lung, intestine, skin, larynx, breast, bladder, prostate and ovary. In this work, the stopping power is calculated by considering the number of velocity-dependent effective charge and effective mean excitation energies of the target material. We used the Hartree-Fock-Roothaan (HFR) atomic wave function to determine the charge density and the continuous slowing down approximation (CSDA) method for the calculation of the proton range. Electronic stopping power values of tissues results have been compared with the ICRU 44, 46 reports, SRIM, Janni and CasP data over the percent error rate. Range values relate to tissues have compared the range results with the SRIM, FLUKA and Geant4 data. For electronic stopping power results, ICRU, SRIM and Janni's data indicated the best fit with our values at 1–50, 50–250 MeV and 250 MeV–1 GeV, respectively. For range results, the best accordance with the calculated values have been found the SRIM data and the error level is less than 10% in proton therapy. However, greater 30% errors were observed in the 250 MeV and over energies.

1. Introduction

The stopping power and range calculations for charged particles in matter have been a topic of long-lasting experimental and theoretical interest. In radiation physics, chemistry, medicine, microdosimetry, proton therapy and biology, it is often required to have simple but accurate information about the stopping power and range values for protons (Tan et al., 2010). Proton beams are used in radiotherapy for effectual cure of tumors. The exact dosimetry of proton radiation depends on comprehensive information about stopping power and range values for proton in the material of interest (Hanson et al., 1981, 1982; Scholz and Kraft, 1996; Schaffner and Pedroni, 1998; Shchemelinin et al., 2002; Dawidowska et al., 2014; Jia et al., 2014). Especially one must know stopping power and range data for the characterization of phantom materials and radiation detector materials (ICRU, 1989).

Many scientist have studied the stopping power and range for proton in several organic materials (Thwaites, 1985; Ashley, 1991; Akkerman et al., 2001; Tan et al., 2006, 2008, 2010; Emfietzoglou et al., 2009; Tan and Liu, 2013; Tufan et al., 2013). However, the stopping power and range data including tissues are scarce, thus, the stopping power and range information of body tissues for protons are needed particularly in proton therapy.

The stopping power of a matter is described as the average energy loss per unit path length and the total stopping power (S_{tot}) is the sum of electronic (S_{el}) and nuclear (S_{nuc}) components:

$$S_{tot}(E) = S_{el}(E) + S_{nuc}(E) \quad (1)$$

For protons, the main contribution to the total stopping power is provided by the electronic stopping power which based on inelastic collisions with target's electrons. Conversely, the least contribute to the total stopping power comes from nuclear stopping power which arise from elastic Coulomb collisions with target's nucleons and is only significant at very low energies. For instance, the nuclear stopping power conduces more than one percent to the total stopping power only at energies below 20 keV for protons in water (ICRU, 1993).

The range (R) is referred to as the travelled distance by the incident particle in target material. The range values are also determined as the distance between the starting point of surface of target and 80% of Bragg peak in proton therapy.

The range of the particle in the target material can be calculated by using continuous slowing down approximation (CSDA) or straight-

* Corresponding author.
E-mail address: musta280@gmail.com (M. Usta).

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Table 1
The elemental compositions and mass densities of some human tissues.

Tissues	Compositions									ρ(g/cm^3)
	H	C	N	O	Na	P	S	Cl	K	
Lung[a]	10.30	10.50	3.10	74.90	0.20	0.20	0.30	0.30	0.20	1.050
Breast[a]	10.60	33.20	3.00	52.70	0.10	0.10	0.20	0.10	–	1.020
Prostate[b]	9.76	9.11	2.47	78.10	0.21	0.10	–	–	0.20	1.045
Bladder[c]	10.50	9.60	2.60	76.10	0.20	0.20	0.20	0.30	0.30	1.040
Skin[a]	10.00	20.40	4.20	64.50	0.20	0.10	0.20	0.30	0.10	1.090
Intestine[a]	10.60	11.50	2.20	75.10	0.10	0.10	0.10	0.20	0.10	1.030
Ovary[a]	10.50	9.30	2.40	76.80	0.20	0.20	0.20	0.20	0.20	1.050
Larynx[a]	10.20	14.30	3.40	71.00	0.10	0.20	0.30	0.10	0.40	1.050

[a] ICRU 44
[b] ICRP 23
[c] ICRU 46

Table 2
Electronic stopping power values for protons in several tissues.

Energy (MeV)	Stopping Power (MeV cm^2/g)							
	Lung	Intestine	Skin	Larynx	Breast	Bladder	Prostate	Ovary
1	2.287E+02	2.307E+02	2.303E+02	2.294E+02	2.368E+02	2.294E+02	2.26E+02	2.294E+02
2	1.480E+02	1.491E+02	1.485E+02	1.482E+02	1.517E+02	1.484E+02	1.47E+02	1.484E+02
3	1.115E+02	1.123E+02	1.119E+02	1.117E+02	1.142E+02	1.118E+02	1.11E+02	1.118E+02
4	9.075E+01	9.130E+01	9.103E+01	9.087E+01	9.271E+01	9.096E+01	8.99E+01	9.097E+01
5	7.701E+01	7.746E+01	7.720E+01	7.710E+01	7.853E+01	7.719E+01	7.64E+01	7.720E+01
6	6.714E+01	6.751E+01	6.726E+01	6.719E+01	6.835E+01	6.729E+01	6.66E+01	6.729E+01
7	5.965E+01	5.997E+01	5.973E+01	5.968E+01	6.065E+01	5.978E+01	5.92E+01	5.979E+01
8	5.375E+01	5.403E+01	5.380E+01	5.378E+01	5.459E+01	5.387E+01	5.33E+01	5.387E+01
9	4.897E+01	4.922E+01	4.901E+01	4.899E+01	4.970E+01	4.908E+01	4.86E+01	4.909E+01
10	4.502E+01	4.525E+01	4.504E+01	4.503E+01	4.566E+01	4.512E+01	4.47E+01	4.513E+01
20	2.546E+01	2.558E+01	2.545E+01	2.546E+01	2.575E+01	2.551E+01	2.53E+01	2.552E+01
30	1.807E+01	1.815E+01	1.806E+01	1.807E+01	1.826E+01	1.811E+01	1.79E+01	1.811E+01
40	1.413E+01	1.419E+01	1.412E+01	1.413E+01	1.427E+01	1.416E+01	1.40E+01	1.416E+01
50	1.166E+01	1.171E+01	1.165E+01	1.166E+01	1.178E+01	1.168E+01	1.16E+01	1.169E+01
60	9.957E+00	1.000E+01	9.948E+00	9.954E+00	1.006E+01	9.978E+00	9.89E+00	9.980E+00
70	8.710E+00	8.747E+00	8.702E+00	8.707E+00	8.793E+00	8.728E+00	8.65E+00	8.729E+00
80	7.753E+00	7.787E+00	7.746E+00	7.751E+00	7.827E+00	7.770E+00	7.70E+00	7.771E+00
90	6.996E+00	7.026E+00	6.989E+00	6.994E+00	7.061E+00	7.011E+00	6.95E+00	7.011E+00
100	6.380E+00	6.407E+00	6.373E+00	6.378E+00	6.439E+00	6.393E+00	6.34E+00	6.394E+00
150	4.468E+00	4.486E+00	4.463E+00	4.466E+00	4.508E+00	4.477E+00	4.44E+00	4.478E+00
200	3.465E+00	3.479E+00	3.461E+00	3.463E+00	3.495E+00	3.472E+00	3.44E+00	3.472E+00
300	2.417E+00	2.427E+00	2.414E+00	2.416E+00	2.437E+00	2.422E+00	2.40E+00	2.422E+00
400	1.870E+00	1.877E+00	1.867E+00	1.869E+00	1.885E+00	1.874E+00	1.86E+00	1.874E+00
500	1.531E+00	1.537E+00	1.529E+00	1.531E+00	1.544E+00	1.534E+00	1.52E+00	1.534E+00
600	1.300E+00	1.305E+00	1.298E+00	1.299E+00	1.310E+00	1.303E+00	1.29E+00	1.303E+00
700	1.132E+00	1.136E+00	1.130E+00	1.131E+00	1.141E+00	1.134E+00	1.12E+00	1.134E+00
800	1.004E+00	1.008E+00	1.002E+00	1.003E+00	1.012E+00	1.006E+00	9.97E−01	1.006E+00
900	9.024E−01	8.520E−01	9.012E−01	9.020E−01	9.095E−01	9.043E−01	8.97E−01	9.043E−01
1000	8.202E−01	7.031E−01	8.134E−01	8.205E−01	8.270E−01	8.222E−01	8.15E−01	8.223E−01

ahead approximation (SAA). In this study we used CSDA method which is based on the assumption that energy of charged particles is lost permanently along their tracks at a rate given by the total stopping power (ICRU, 1993).

In the present study, we supplied the tables for the electronic stopping power and range values of protons incident on the 8 selected human tissues over energies ranging from 1 MeV to 1 GeV. The considered human tissues are lung, intestine, skin, larynx, breast, bladder, prostate and ovary. The elemental compositions and the density information of these tissues were taken from ICRU 44–46 (ICRU, 1989, 1992) and ICRP 23 (ICRP, 1975) reports. We followed the procedure in Ref. (Tufan et al., 2005) to compute the stopping power and considered only electronic energy loss since the contribution to the total stopping power from the nuclear interactions is quite small at medium and high energy. Moreover, we have used the Hartree-Fock-Roothaan (HFR) atomic wave functions (Bunge et al., 1993) to determine the charge density. This study is the first application of HFR charge density to the range and stopping power calculations.

The object of this work is to present the consequences for the stopping power and range values of some human tissues at energies ranging from 1 MeV to 1 GeV and 1–500 MeV, respectively. The obtained results were compared with literature and listed in the Tables. These results can be used as a reference data in many dosimetry problems and proton therapy.

2. Material and methods

2.1. Electronic stopping power calculations

In this work, the stopping power is calculated by considering the number of velocity-dependent effective charge and effective mean excitation energies of the target material (Tufan et al., 2005).

Interaction potential between proton and target can be written as

$$V(\mathbf{x}, \mathbf{y}, \mathbf{R}) = \frac{Ze^2}{\mathbf{R}} - \sum_{i=1}^{Z^*} \frac{e^2}{|\mathbf{R} - \mathbf{y}_i|} \quad (2)$$