Mass Stopping Power of Methanol and Methanal for Boron and Carbon Ions Using Relativistic Bethe Equation

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Abstract:

The calculation of the mass stopping power of two organic compounds (Methanol and Methanal) for boron and carbon ions performed in the energy range (10^{-2}-10^3 MeV) using relativistic Bethe equation, which has been programmed using MATLAB2021. And the curve fitting was used, and the calculated results were compared with the empirical data of the SRIM-2013 program for the same projectiles in the same organic compounds. The theoretical results calculated showed good agreement with the empirical data in the high energies region.

INTRODUCTION

Niels Bohr published a seminar paper on the theory of charged particle penetration in the matter, which was purely based on classical physics. It is instructive to look at Bohr's earlier work because it represents the first attempt at a unified theory of stopping.[1].He assessed the classical stopping of an electron bound in a harmonic potential by a fast heavy charged particle. [2]. Think about a charged particle entering a kinetically active medium. The "Range" is then the average value of the distances a particle travels before coming to rest. Due to multiple coulomb scattering, a proton's range in an absorbing medium will be somewhat smaller than the path length calculated from the initial angle of incidence into the material. [3]. As is well known, charged particles passing through a material medium experience some kinetic energy loss whenever they collide with a target material. The process of charged particles moving through a medium with constant kinetic energy until their kinetic energy is zero, at which point they lose all of their energy and come to rest. The total range for charged particles passing in the

material medium can therefore be defined as the distance the particle travels before it reaches the rest, depending on the matter target, the type of incident particle, as well as its energy. [4]. Many authors, including Livingston and Bethe, Sternheiner, Bichsel, etc., have found range-energy relations for protons. Sternheimer made an estimate. [5] for proton energies between 2 MeV and 100 GeV, to determine range energy relations for some of the commonly used materials, including aluminum, copper, carbon, beryllium, and lead. For the same substances, Bichsel has also discovered a range energy relation between 1 MeV and 100 MeV [6].

STOPPING POWER FORMALISM

An accelerating beam traversing the target would be energy inefficient. This energy loss is attributed to the dispersion of electrons and nuclei, with the electronic stopping force being the most significant in nearly all energy domains. In particular, the beam speed has an impact on the energy loss. Typically, the energy loss at a given power is expressed in terms of stopping power, which can be defined as the energy loss per given volume of material. A medium's stopping power is the energy loss rate for a particle per unit length of its path. Utilizing the relativistic Bethe formula as [7].

$$-\frac{dE}{dX} = \left(\frac{ze^2}{4\pi\varepsilon_.}\right)^2 \frac{4\pi Z\rho N_A}{Ame^2}\left[\ln\left(\frac{2mv^2}{I}\right) - \ln(1-\beta^2) - \beta^2\right] \tag{1}$$

Where $v = \beta c$, is the ion velocity, ze, ion charge, m, electron mass, I, mean ionization energy of elements, N_A, Avogadro's number, A, the mass number of the element, Z, the atomic number of the element, ρ, target density [7].

Depending on the projectile charge and the target material, the stopping power is expressed as the energy loss per distance in the target material (-dE/dx) [8]. One of the topics that takes up a lot of space in physics scientists' research is the study of stopping power. These studies employed a variety of techniques and were both theoretical and experimental [9]. The Bragg additive rule is found to function quite well for compounds. According to the rule, a substance's mass-stopping power is equal to the weighted sum of its constituent atoms' mass-stopping powers [10].

$$\left(\frac{-dE}{\rho dx}\right)_{com} = \sum_i \omega_i \left(\frac{-dE}{\rho dx}\right)_i \tag{2}$$

where ω_i : the ratio of the atomic weight of the elements in the compound,

$$\omega_i = \frac{n_i A_i}{A_{comp}} \tag{3}$$

n_i : atoms number., A_i: atomic mass of elements in medium, A_{comp} : atomic mass of medium, $\left(\frac{-dE}{\rho dx}\right)_{com}$: Mass stopping power of compound, $\left(\frac{-dE}{\rho dx}\right)_i$:stopping power Mass for the elements in the compound.

RESULTS AND DISCUSSION

In the beginning, the atomic weight ratios were calculated for each organic compound's components, composed of hydrogen, carbon, and oxygen, using Eq. 3, as listed in Table 1. The mass   stopping power of heavy charged particles (boron and carbon ions) was calculated in targets (methanol CH_3OH, methanal CH_2O) as shown in Table 2 based on the Beth-Relativistic Equation (Eq. 1) with an energy range of (0.01-1000 MeV) and programmed using the Matlab2021 program, the calculated results were compared with the practical results of the global code SRIM2013, and it showed good agreement at high energies.

TABLE 1: Atomic weight ratios of Methanol CH_3OH and Methanal CH_2O.

Organic compound	Atomic weight ratios ω_i		
	H	C	O
Methanol CH_3OH	0.126	0.375	0.499
Methanal CH_2O	0.067	0.400	0.533

In Table 1 and Figure 1, and Figure 2, calculations of the stopping power of the boron ion B^{+5} and the carbon ion C^{+6} were calculated in two organic compounds (methanol and methanal) within the energy range (0.01-1000 MeV). It has negative values at energies (0.01-0.4 MeV). The negative sign is attributed to the logarithm in Eq. 1. And these negative values do not make sense physically, as they mean that the energy of the projectile increases whenever it passes inside the porous media, and this contradicts the reality, as whenever the projectile moves inside the porous media (targets), it loses its energy until it reaches a state of rest. In this case, the negative values of the stopping power are neglected. At energies (E > 0.3 MeV) for boron ion, the calculated stopping

power increases until it reaches its greatest value at 1 MeV for methanal and 0.9 MeV for methanol. For carbon ions, the calculated stopping power increases until it reaches its maximum value at 1 MeV for methanol and methanol. The highest value of mass stopping power is attributed to the ionization and irritation of the atoms of the organic compounds that represent the porous media. After that, the stopping power of the carbon ion shells begins to decrease in all media. The electronic effect at high energies dominates it.

TABLE 2: Calculations of Mass stopping power of Methanol and Methanal for Boron and Carbon ions.

| Energy (MeV) | Boron Ions (B^{+5}) | | | | Carbon Ions (C^{+6}) | | | |
| | β^2 | v (m/sec) | Mass Stopping Power (MeV cm²/g) | | β^2 | v (m/sec) | Mass Stopping Power (MeV cm²/g) | |
			Methanol	Methanal			Methanol	Methanal
0.01	0.000002	422777.21	-7557719.93	-7489309.07	0.000002	401285.91	-12442201.97	-12314230.51
0.02	0.000004	597896.82	-3026286.91	-3030786.17	0.000004	567503.59	-5018208.71	-5016087.47
0.03	0.000006	732270.51	-1724040.75	-1742134.15	0.000005	695046.65	-2876375.81	-2899087.28
0.04	0.000008	845552.53	-1136858.31	-1158460.34	0.000007	802570.20	-1907660.33	-1937532.02
0.05	0.000010	945355.76	-812577.52	-834843.22	0.000009	897300.16	-1371231.32	-1403095.08
0.06	0.000012	1035584.58	-611164.25	-633112.59	0.000011	982942.42	-1037226.22	-1069203.56
0.07	0.000014	1118558.35	-476036.48	-497308.70	0.000013	1061698.44	-812619.10	-843959.21
0.08	0.000016	1195788.29	-380287.40	-400764.69	0.000014	1135002.62	-653109.45	-683511.56
0.09	0.000018	1268324.07	-309615.54	-329279.14	0.000016	1203851.26	-535119.65	-564479.86
0.1	0.000020	1336929.96	-255775.55	-274649.46	0.000018	1268969.80	-445039.41	-473344.36
0.2	0.000040	1890690.40	-52631.25	-65938.85	0.000036	1794582.26	-102231.82	-122570.98
0.3	0.000060	2315596.12	-5739.12	-16120.39	0.000054	2197890.67	-21245.04	-37217.25
0.4	0.000079	2673800.18	11313.12	2723.85	0.000072	2537888.51	9028.60	-4234.52
0.5	0.000099	2989377.21	18741.75	11371.82	0.000089	2837426.58	22712.98	11305.69
0.6	0.000119	3274674.28	22216.87	15735.82	0.000107	3108224.23	29474.61	19425.99
0.7	0.000139	3537026.14	23825.28	18024.08	0.000125	3357243.36	32907.65	23901.34
0.8	0.000159	3781211.84	24471.97	19209.43	0.000143	3589020.04	34587.94	26409.36
0.9	0.000179	4010550.93	24595.03	19770.99	0.000161	3806705.07	35287.56	27784.01
1	0.000199	4227460.39	24423.76	19964.39	0.000179	4012592.55	35416.14	28474.78
2	0.000397	5978086.66	19740.10	17123.01	0.000358	5674282.12	29740.35	25650.51
3	0.000596	7321085.87	16097.13	14201.19	0.000537	6949081.78	24520.90	21552.70
4	0.000794	8453032.48	13636.51	12134.02	0.000715	8023570.30	20889.56	18534.73
5	0.000992	9450074.17	11880.01	10627.99	0.000894	8970022.71	18262.99	16299.20
6	0.001191	10351267.13	10561.38	9483.94	0.001073	9825508.67	16275.95	14584.99
7	0.001389	11179814.34	9532.19	8583.94	0.001251	10612050.75	14717.07	13228.17
8	0.001587	11950834.96	8704.39	7855.90	0.001430	11343998.88	13458.54	12125.78
9	0.001785	12674831.59	8022.59	7253.65	0.001608	12031321.24	12419.01	11210.81
10	0.001983	13359451.70	7450.21	6746.29	0.001787	12681276.07	11544.32	10437.99
20	0.003960	18879076.70	4483.86	4092.64	0.003569	17922022.41	6983.71	6367.89
30	0.005932	23104888.25	3287.41	3011.10	0.005346	21935220.76	5131.48	4696.25
40	0.007897	26659445.05	2625.52	2409.94	0.007119	25311684.24	4103.57	3763.86
50	0.009857	29784090.80	2200.52	2022.82	0.008886	28280430.66	3442.26	3162.15
60	0.011810	32602700.67	1902.53	1750.82	0.010650	30958999.07	2977.93	2738.77
70	0.013758	35188920.82	1681.01	1548.33	0.012408	33417262.95	2632.41	2423.21
80	0.015701	37590773.94	1509.34	1391.20	0.014162	35700781.21	2364.41	2178.13
90	0.017637	39841643.27	1372.06	1265.43	0.015911	37841221.81	2149.96	1981.82
100	0.019568	41965854.41	1259.58	1162.29	0.017655	39861658.51	1974.14	1820.73
200	0.038567	58915821.21	715.01	661.75	0.034847	56001720.03	1121.45	1037.49
300	0.057020	71636500.02	513.27	475.71	0.051591	68140808.10	804.80	745.66
400	0.074946	82128843.72	406.30	376.92	0.067903	78174599.99	636.69	590.45
500	0.092366	91175292.59	339.51	315.16	0.083798	86843616.26	531.60	493.33
600	0.109298	99180892.66	293.63	272.71	0.099290	94530822.79	459.37	426.52
700	0.125761	106388510.57	260.08	241.64	0.114392	101465625.16	406.50	377.59
800	0.141772	112957862.11	234.43	217.88	0.129117	107798746.27	366.07	340.15
900	0.157347	119000911.94	214.15	199.10	0.143479	113635752.85	334.09	310.52
1000	0.172502	124599925.12	197.71	183.86	0.157488	119054144.41	308.14	286.48
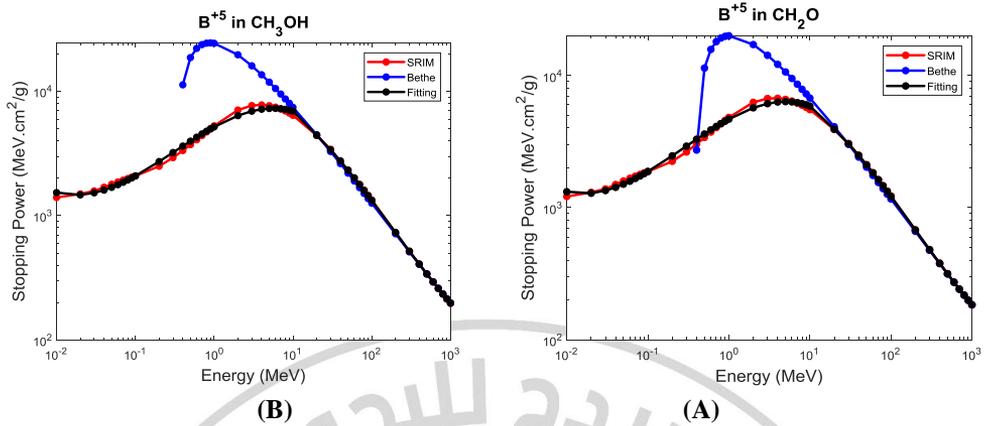
FIGURE 1: Mass stopping power of (A) Methanol CH₃OH, (B) Methanal CH₂O for boron ion.

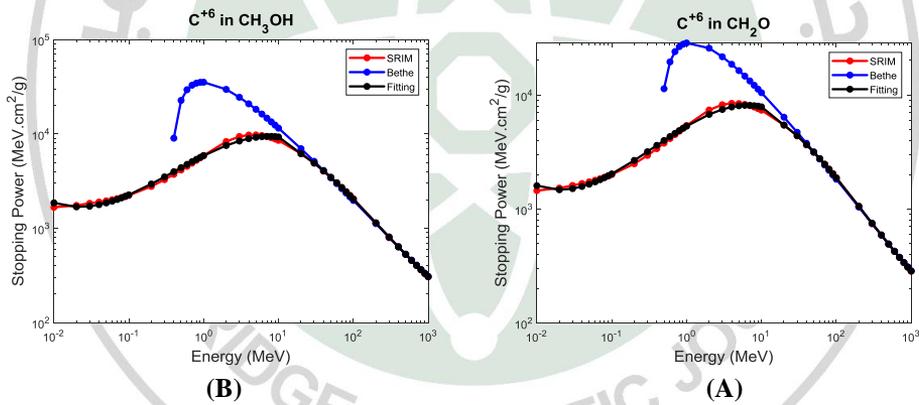**FIGURE 2: Mass stopping power of (A) Methanol CH₃OH, (B) Methanal CH₂O for carbon ion.**

CONCLUSIONS

The most important conclusions were reached by writing the relative Beth equation and the associated equations in the MATLAB 2021 accredited mathematical program, where the mass-stopping ability of the relative heavy ions in the studied organic compounds was studied, and the following was concluded:

1. Though it requires some adjustments at low energies for its results to be in good agreement with those of the international code SRIM2013, the relativistic Bethe equation is very suitable for determining the stopping power of relative heavy ions in the studied organic compounds.

2. The maximum value of the mass stopping power is at low or medium energies and decreases gradually with increasing energy.

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خلاصة بحث النشر

Abstract:

The calculation of the mass stopping power of two organic compounds (Methanol and Methanal) for boron and carbon ions performed in the energy range (10^{-2}-10^3 MeV) using relativistic Bethe equation, which has been programmed using MATLAB2021. And the curve fitting was used, and the calculated results were compared with the empirical data of the SRIM-2013 program for the same projectiles in the same organic compounds. The theoretical results calculated showed good agreement with the empirical data in the high energies region.

خلاصة

تم حساب قدرة الإيقاف الكتلية لمركبين عضويين (ميثانول ,ميثانال) لأيونات البورون والكربون تم اجراؤها ضمن مدى طاقة MeV (10^3 – 10^{-2}) باستخدام معادلة بيث النسبية والتي تمت برمجتها باستخدام برنامج ماتلاب 2021 , كما وتم استخدام اداة مطابقة المنحني (curve Fitting Toll) وتمت مقارنة النتائج المحسوبة مع البيانات التجريبية لبرنامج SRIM 2013 , لنفس القذائف في نفس المركبات العضوية . اظهرت النتائج المحسوبة نظرياً توافقاً جيداً مع البيانات التجريبية .

الكلمات المفتاحية : قدرة الإيقاف الكتلية , الأيونات الثقيلة , صيغة بيث النسبية , ماتلاب 2021 , برنامج SRIM 2013 , المركبات العضوية .