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Calculating the stopping power of protons and alpha particles in polycarbonate (PC)$C_{16}H_{14}O_3$ and polyurethane (PU)$C_{27}H_{36}N_2O_{10}$

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Abstract:

In this study, the alpha particle in polycarbonate and protons were studied by using the Bethe, Bragg, and Ziegler equations to determine the stopping power of charged particles. $C_{16}H_{14}O_3$ and polyurethane $C_{27}H_{36}N_2O_{10}$over the energy spectrum from 0.01 to 1000 MeV. The Bethe equation was found to be well-compatible with the experimental data in the medium and high energy area when the calculations were compared with the data from P-STAR, SRIM 2013, and A-STAR. The equations were coded in MATLAB 2021. The findings also shown that, across all energy ranges, the stopping power computed using the Ziegler equations agrees well with experimental data. There was a 0.9 correlation coefficient. The significance of these targets in the chemical and industrial domains led to their selection.

Keywords: Stopping Power, P-star, A-star, Srim 2013, Bethe, Ziegler, Bragg base

1. Introduction

A large number of physicists have made theoretical and practical attempts to examine the problem of halting ability calculation. Interactions between the atoms of matter-containing charged particles produce electromagnetic forces between the particles. The elastic and inelastic components of this interaction are distinct from one another. The nuclear stopping power is the rate of the percentage of energy lost during a flexible reaction, while the electronic stopping power is the rate of the percentage of energy lost from an inflexible reaction. In a flexible reaction, momentum is transferred to the target atom overall, while in an inflexible reaction, the ionization of the target atoms results in the rate of the percentage of energy lost [1].The energy of the charged particle will be steadily depleted as it travels through the material along its continuous route. Once its power is depleted, it comes to a halt. The route length or range is the amount of distance a particle travels before coming to a halt. The particle's kinetic energy is completely used up at the end of its range, and the distance it travels through the material is dependent on the target's material properties [2]. Prior to Betz's explanation, it was believed that the observed charge states of ions leaving gaseous targets were much bigger than those leaving solid targets. However, Betz later clarified that ions with almost the same atomic number in gaseous and solid materials had very comparable charge states [3]. In order to better understand the proton shell and its properties, this study will investigate stopping power. alpha particle in polymers $\boldsymbol{C_{27}H_{36}N_2O_{10}}$, $\boldsymbol{C_{16}H_{14}O_3}$ using the Bethe, Ziegler and Bragg equations.

2. Theoretical details

First, as charged particles travel through matter, they lose energy through ionization or excitation of atoms (aside from low-velocity and nuclear collisions). This is because charged particle motion produces an electromagnetic force that the atom's electrons can use, which in turn adds energy to the atom.
leaving an atom in an excited state or ionizing it after removing an electron from it [4]. Both Bohr's (1913) theory of classical mechanics and Bethe's (1930) theory of quantum mechanics are used to determine the stopping power. The stopping power is determined by integrating quantum and classical mechanics using the K_B coefficient, which differentiates between quantum disorder and classical dispersion.
[5], as it is given by K_B =2 Z1Vo\V.

The stopping power, denoted as (dE\dX), is the amount of energy a particle loses for every unit length of its travel through a medium. The projectile's charge, velocity, target material, and unit (MeV. cm^(-1)) determine its stopping power. [6]. Using the Bethe formula, Bichsel determined the stopping power and range ability of fast ions in heavy elements (those with an atomic number of Z<56) in 1992. Compatibility with the empirical values of protons with a power greater than 0.5 MeV was found in the computed stopping and ranging abilities [7]. In 1937, Bethe succeeded in creating a formula for the stopping power that is based on quantum theory, works within the restrictions of high-speed travel, is analogous to the Bohr formula, and changes only in logarithms [8].
The stopping power in compounds is given by the following equation:

$$S_{com}(E) = \sum w_i S_i(E) \qquad (1)$$

where:

$$w_i = \frac{A_i N_i}{\sum A_i N_i} \qquad (2)$$

S_i: the element's repulsion force and Yi: the element's weight ratio in the compound and Nl: the total atomic number of the chemical and Here is the code for the medium's atomic mass and Bethe's equation:

$$\frac{-dE}{\rho dx} = 4\pi \frac{k_o^2 Z_1^2 Z_2 e^4 N_A}{mc^2 \beta^2 A_2}\left[ln\left(\frac{2mc^2\beta^2}{I(1-\beta^2)}\right) - \beta^2\right] \qquad (3)$$

K_o = (K_0=8.99×109 N.m^2\c^2)The given equation can be paraphrased as follows: F m_e is equal to 9.1×10^(-31) kg, 〖mc〗 ^2 is the static energy of the electron, which is 5.11×eV, Z1 is the atomic number of the proton, which is 1, Z2 is the atomic number of alpha particles, which is 2, e is the electron charge, which is 1.6×10^-19 C, c is the speed of light in space, which is 3108 m/sec, NA is the Avcadro number, which is 6.02×10^23 mol, β is the relative speed, which is equal to (β=v/c), and I is the average ionization voltage, which is in e

:

$$\beta^2 = 1 - \frac{1}{(1 + \text{Ep}\backslash 931.5\ M_1)^2} \qquad (4)$$

M_1The unit of atomic mass is (1.008) for a proton and (4.002) for an alpha particle. Since the electrical configuration and physical state of molecules or atoms in the stopping medium are essential factors in theoretical estimates of the stopping power, the rate of ionization voltage is also an important variable to consider [9]. It is defined as being lower than the amount of energy needed to remove an electron from its orbit when it is bound to another electron. The polarization, stopping cross-section, stopping power, chemical formula, and concentration of substances (solid, liquid, or gas) are among the several atomic parameters that determine the ionization voltage [10]. By using quantum mechanics and determining the Bethe equation for various elements, the ionization voltage rate may be determined. If you know the atomic number (Z) of an element, you may use approximate empirical methods like these to estimate its I value in units (eV) [11].

$$I = \begin{cases} 19.2 & eV & if\ \ z2 = 1 \\ 11.2 + 11.7 & eV & if\ 2 \le z2 \le 13 \\ 52.8 + 8.71z2 & eV & if\ \ z2 > 13 \end{cases} \qquad (5)$$

The Ziegler equations for the proton are written as follows:

2.1. Electronic stopping power equations

If power range (10^{-3}-10^{-2}MeV) equation used:

$$S_e = A_1 E^{\frac{1}{2}} \qquad (6)$$

If the power is in the range of ($0.0999-10^{-2}$ MeV) Equation used:

$$S_e = \frac{S_{low} S_{high}}{S_{low} + S_{high}} \qquad (7)$$

where:

$$S_{low} = A_2 E^{0.45} \qquad (8)$$

$$S_{high} = \frac{A_3}{E} ln\left[1 + \frac{A_4}{E} + \frac{A_5}{E}\right] \qquad (9)$$

If power range (1-10^3MeV) Equation used:

$$S_e = \frac{A_6}{\beta^2}[\ln(A_7\beta^2)/1 - \beta^2] - \beta^2 - \sum_{i=0}^{4} A_{i+8}(\ln(E))^i \qquad (10)$$

2.2. Nuclear stopping power Equations

If the energy is E≤ 0.03 MeV Equation used:

$$S_n = \frac{\ln(1 + 1.1383\varepsilon)}{2(\varepsilon + 0.1231\varepsilon^{0.21226} + 1.9593\varepsilon^{0.5})} \qquad (11)$$

If energy E> 0.03 *MeV is the equation used:*

$$S_n = \frac{\ln(\varepsilon)}{2\varepsilon} \qquad (12)$$

where:

$$\varepsilon = \frac{32.53 M_2 E}{Z_1 Z_2 (M_1 + M_2)(Z_1^{0.23} + Z_2^{0.23})} \qquad (13)$$

The alpha particle's Ziegler equations are expressed in the following way:
1-Nuclear Stopping Power Equations:

$$\varepsilon = \frac{32.53 M_2 E}{Z_1 Z_2 (M_1 + M_2)\left(Z_1^{\frac{2}{3}} + Z_2^{\frac{2}{3}}\right)^{1/2}} \qquad (14)$$

If ($\varepsilon < 0.01$) the equation used:

$$S_{nz} = 1.593\varepsilon^{1/2} \qquad (15)$$

When the energy is ($0.01 \le \varepsilon \le 10$) the equation used: $S_{nz} = 1.7(\varepsilon^{1/2})[\ln(\varepsilon + exp1) / 1 + 6.8\varepsilon + 3.4\varepsilon^{3/2}]$ (16)

If ($\varepsilon > 10$) the equation used:

$$S_{nz} = \frac{ln(0.47\varepsilon)}{2\varepsilon} \qquad (17)$$

2-Electronic Stopping Power Equations:

If the energy ($E \le 10^4$):

$$S_e = \frac{S_{low} S_{high}}{S_{low} + S_{high}} \qquad (18)$$

where:

$$S_{low} = A_1 E^{A2} \qquad (19)$$

$$S_{high} = \frac{1000A_3}{E} \ln\left(1 + \frac{1000A_4}{E} + \frac{A_5 E}{1000}\right) \qquad (20)$$

If energy ($E > 10^4$) is the equation used:

$$S_{ez} = \exp\left(A_6 + A_7 \ln\left(\frac{1000}{E}\right) + A_8 \ln\left(\frac{1000}{E}\right)^2 + A_9 ln\left(\frac{1000}{E}\right)^3\right) \qquad (21)$$

3. Results and discussion

The mass stopping power of protons and alpha particles was calculated as shown in the tables (1),(2).

Table (1) displays the outcomes of the proton stopping power employed in the polymers ($C_{16}H_{14}O_3, C_{27}H_{36}N_2O_{10}$)

E_{proton} (MeV)	PC				PU			
	Bethe	Zeigler	P-star	SRIM	Bethe	Zeigler	P-star	SRIM
0.01	-9178.08	510.67	500.27	483.31	-9295.27	520.32	512.86	481.27
0.1	824.08	866.00	858.56	841.86	829.90	888.01	882.63	851.25
1	256.88	255.44	249.43	247.80	259.22	260.54	253.19	248.11
10	43.65	44.34	43.74	44.19	44.06	45.04	44.26	44.66
50	11.82	12.04	11.89	11.97	11.94	12.22	12.03	12.09

100	6.92	7.04	6.95	7.00	6.98	7.13	7.04	7.07
150	5.17	5.25	5.19	5.22	5.22	5.32	5.25	5.28
200	4.26	4.32	4.28	4.30	4.30	4.38	4.33	4.35
225	3.95	4.01	3.97	3.99	3.99	4.07	4.02	4.03
250	3.71	3.76	3.72	3.74	3.74	3.81	3.77	3.78
275	3.51	3.56	3.52	3.54	3.54	3.60	3.56	3.57
300	3.34	3.38	3.35	3.36	3.37	3.43	3.39	3.40
350	3.07	3.11	3.08	3.09	3.10	3.16	3.12	3.13
400	2.88	2.91	2.88	2.89	2.90	2.95	2.92	2.93
450	2.72	2.76	2.72	2.74	2.75	2.79	2.76	2.77
500	2.60	2.63	2.60	2.61	2.63	2.67	2.63	2.64
550	2.50	2.53	2.50	2.51	2.53	2.57	2.53	2.54
600	2.42	2.45	2.42	2.43	2.45	2.49	2.45	2.46
650	2.36	2.39	2.35	2.36	2.38	2.42	2.38	2.39
700	2.30	2.33	2.29	2.30	2.32	2.36	2.32	2.33
800	2.21	2.24	2.20	2.21	2.23	2.27	2.23	2.24
900	2.15	2.17	2.13	2.14	2.17	2.20	2.16	2.17
1000	2.10	2.12	2.08	2.09	2.12	2.15	2.11	2.12

Table (2) the end product of alpha particle kinetic energy in *polymers*($C_{16}H_{14}O_3, C_{27}H_{36}N_2O_{10}$).

E_{alpha}	PC				PU			
(MeV)	Bethe	Zeigler	A-star	SRIM	Bethe	Zeigler	A-star	SRIM
0.01	-311400.	521.81	569.37	521.21	-314929	492.12	547.44	502.81
0.1	-3478.23	1289.64	1370.20	1299.37	-3552.57	1250.45	1356.60	1271.85
1	2418.96	1944.47	2091.62	2048.20	2439.38	1951.79	2156.31	2082.26

10	520.07	519.62	512.97	530.82	524.92	525.45	519.54	537.48
50	144.75	149.65	145.23	147.38	146.13	151.83	146.96	148.96
100	82.24	85.70	82.69	83.64	83.03	87.08	83.66	84.51
150	59.20	62.10	59.55	60.14	59.76	63.17	60.24	60.77
200	47.01	49.61	47.29	47.73	47.46	50.50	47.84	48.23
225	42.82	45.31	43.09	43.46	43.23	46.14	43.59	43.92
250	39.42	41.81	39.66	40.00	39.80	42.59	40.12	40.42
275	36.60	38.90	36.82	37.12	36.95	39.64	37.25	37.51
300	34.21	36.44	34.42	34.70	34.54	37.14	34.82	35.07
350	30.41	32.50	30.60	30.83	30.71	33.15	30.95	31.16
400	27.51	29.48	27.68	27.89	27.78	30.08	28.00	28.18
450	25.23	27.09	25.37	25.56	25.47	27.65	25.67	25.83
500	23.37	25.14	23.50	23.67	23.60	25.67	23.78	23.92
550	21.84	23.52	21.96	22.11	22.05	24.03	22.22	22.35
600	20.55	22.15	20.67	20.80	20.75	22.64	20.91	21.02
650	19.46	20.98	19.56	19.69	19.65	21.44	19.79	19.90
700	18.51	19.96	18.61	18.73	18.69	20.41	18.83	18.93
800	16.96	18.27	17.04	17.15	17.13	18.70	17.24	17.33
900	15.75	16.94	15.82	15.91	15.90	17.34	16.01	16.09
1000	14.77	15.85	14.83	14.92	14.91	16.23	15.00	15.08

Within the energy range of 0.01 to 1000 MeV, the polymer's proton stopping power (C_16 H_14 O_3, C_27 H_36 N_2 O_10) was determined. The Bethe and Ziegler equations were used to compute the values of the components C, H, O, and N separately. The Bragg equation was then applied to the polymer. All of the aforementioned equations were coded in MATLAB 2021. The findings of the SREM2013 program and the P-STAR utilizing the MATLAB2021 software are compared using the previously mentioned equations in Figures (1, 3), which theoretically estimate the values of the stopping powers as a function of proton energy.

The Bethe equation, when used, yields negative values for the stopping power at low energies, where the cut occurs between 0.01 and 0.03 MeV.

which is the upper limit in Figure (1). The energy range from 0.01 MeV to 0.03 MeV is the cutoff limit shown in Figure 3. The explanation for the negative value is the logarithmic meaning of the shell, which means it does not have any physical existence. Contrary to reality, everything that enters the material instead of slowing it down enhances speed. The logarithm in the Bethe equation causes a cutoff process, and these energies are the cutoff for these negative consequences. Another premise upon which Bethe's theory rests is that the falling particle's velocity is much higher than the motion of the orbital electrons of the atoms in the target material. Figure 1 shows the results of using the Bethe equation, which yielded the highest proton stopping power value. Energy E=0.09 MeV is its value. The maximum stopping power value is shown in Figure (3) with an energy of E=0.1 MeV. Atomic ionization and excitation provide the strongest stopping power. The stopping power drops down sharply when the particle's kinetic energy rises over these upper limits. When the Bethe equation is used, the energy quickly decreases since it is inversely proportional to the square of the falling particle's velocity (1\v2) or, conversely, to the projectile's energy. Electronic deactivation is the main phenomenon at these energies. As a result of the quantitative nature of the Bethe equation, which is well-suited to high energies, we find that its results differ significantly from the SREM2013 and P-STAR programs' empirical values at low energies, but agree with them at high energies.
The stopping power of protons was calculated using Ziegler's equations in a three-zone energy model: in the low-energy zone (E >10 MeV), as shown in Figures (1,3), the values of the stopping power are low and increase slowly because the particle is moving at a low speed; furthermore, nuclear collisions are common in this region.In regards to the medium energy region (10>E>100 MeV), it can be shown from Figures (1,3) that the stopping power has increased and reached its maximum Because the atoms of the substance have been excited and ionized, their stopping power has grown and reached its maximum.
subject matter in this domain.Consistent with the findings of SREM2013 and P-STAR, Figure (1) shows that the stopping power is highest at an energy of 0.1 MeV, and Figure (3) shows that it is highest at an energy of 0.08 MeV. Because energy loss is inversely proportional to the square of the particle's velocity, we can infer from Figures (1,3) that in the high energy areas, MeV (100>E>1000), the stopping power peaks in

the medium energy area and then begins to decline as the falling particle's energy increases.

. This is when electronic halting becomes the norm. In order to find the stopping power levels, the correlation coefficient Rc was calculated using SREM2013 data, Ziegler equations, and Bethe's equations. Zeiglerp and SRIM p have P-STAR values of (0.9998) as shown in Figure (3), but P-star and Bethep have P-STAR values of (0.9441) as shown in Figure (1). Using Zeiglerp and SRIM p, the P-STAR values for Figure (3) are (0.9998).

We find out the stopping power of the polymer's alpha particles (C_16 H_14 O_3, C_27 H_36 N_2 O_10) in the energy range of 0.01 to 1000 MeV. After computing the aforementioned equations for each element (C, H, O, and N) independently using the Bethe and Ziegler equations, we programmed them into MATLAB 2021. Next, we used the polymer in the Bragg equation. Comparisons are made between the theoretically calculated values of the stopping power as a function of alpha particle energy using the aforementioned equations in Figures (2, 4), and results obtained using the SREM2013 and A-STAR programs in MATLAB 2021.The Bethe equation yields negative values for the stopping power at low energies, as shown in Figure (2) and Figure (4), respectively, for the cut-off limit, which falls between the energies (0.1 0.01 >E> 0.1 MeV) and MeV (0.01>E>0.09), respectively. The projectile's negative value is due to its logarithmic meaning; therefore, it lacks physical reality. If the material's speed decreases as its composition increases, it will

increase, and this is contrary to reality. A cut- These energies serve as the cutoff for these negative findings, since the logarithm in the It is the Bethe equation that triggers the off process. The fact that the speed of the falling particle is much greater than that of the atoms' orbital electrons in the substance of interest is another assumption upon which Bethe's theory is based. The Bethe equation, as seen in Figure (2), produces the maximum stopping power value for alpha particles with an energy of E=0.3 MeV. Figure 4 shows the greatest stopping power value with an energy of E=0.4 MeV. According to Figure (2), the stopping power of alpha particles, as determined by the Ziegler equations, is at its highest at an energy of E=0.6 MeV, and Figure (4) confirms this with an energy of E=0.8 MeV. These results are promising and corroborate the practical claims made by the SREM2013 and A-STAR initiatives, respectively. With the use of stopping power values calculated from the Bethe equations, Ziegler equations, SREM2013 data, and A-STAR values, the correlation coefficient Rc was finally established. The stopping power at the A-star and Bethe connection was 0.9616

in Figure (2), 0.9995 at the Zeigler and SRIM connection in Figure (3), and 0.9616 at the A-star and Bethe connection in Figure (4).
The value was 0.9610, while the value between Zeigler and SRIM was 0.9994.

Figure 1: Stopping power of the proton in polycarbonate

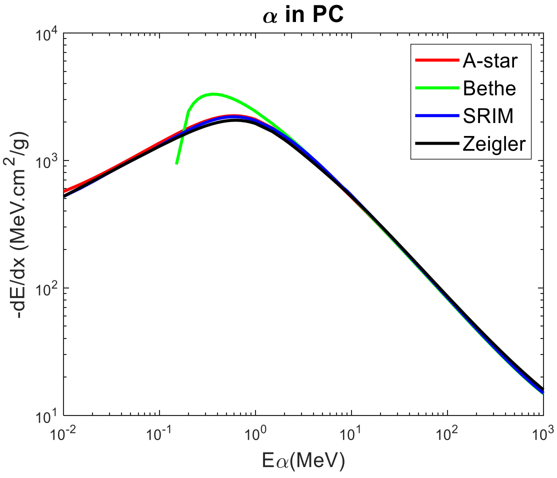

Figure 2: Alpha particle stopping power in polycarbonate

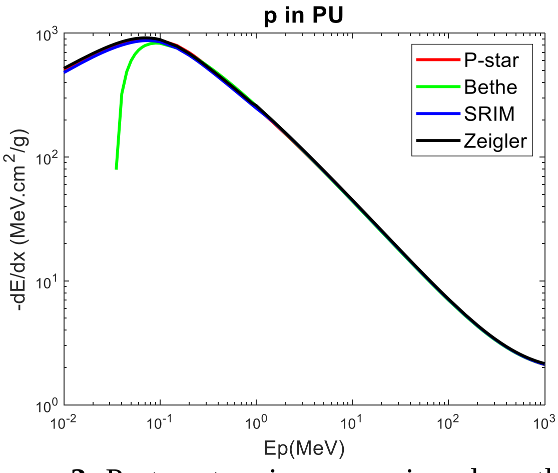

Figure 3: Proton stopping power in polyurethane.

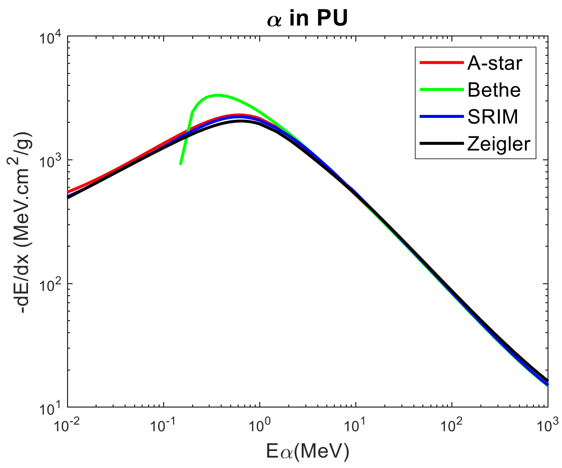

Figure 4: Alpha particle stopping power in polyurethane.

4. Conclusion

Through the results obtained from this study, the following was concluded : Across all power ranges, the stopping power computed using Ziegler's equations agrees well with experimental data.
In the medium and high energy area, this comparison demonstrated that the Bethe equation is well-suited to the available empirical evidence.

It was found that the polymer PC's maximum stopping power value as determined by the Bethe equation is higher than the maximum stopping power value as determined by the Ziegler equation for protons, but for alpha particles, the lowest maximum stopping power value as determined by the Bethe equation is lower than the highest value determined by the Ziegler equation.
When it comes to protons in PU polymers, we discovered that the Bethe equation yields a higher greatest stopping power value than the Ziegler equation, but when it comes to alpha particles, the Bethe equation yields a lower greatest stopping power value.
In accordance with the Bethe equation, the PC polymer exhibits its maximum stopping power for protons at energies ranging from 0.01-0.09 MeV and for alpha particles at energies ranging from 0.01-0.3 MeV. Subsequently, as the projectile energies increase, this stopping power progressively decreases.
Based on the Bethe equation, the studied compounds' PU polymer exhibits its maximum stopping power for protons at energies ranging from 0.01-0.1 MeV and alpha particles at energies ranging from 0.01-0.4 MeV. Subsequently, as the projectile energies increase, this stopping power starts to gradually decrease.

The two polymers show their strongest stopping power at proton energies of (0.01-0.07 MeV) and alpha particle energies of (0.01-0.65 MeV), according to the Ziegler equation for the compounds being studied. after which it starts to fall off steadily as the projectiles' energies rise.

Through the results, we note that the value of the stopping power according to Bethe when the The proton energy is negative at 0.01 MeV, which is equal to -9178.08 MeV for the polymer. Similarly, the stopping power Bethe is -311400 MeV when the particle energy of Alpha is negative at 0.01 MeV. Based on the findings, we may deduce that the Bethe equation does not hold for energies E≤0.01MeV and that the stopping power is negative at 0.01MeV.

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حساب قدرة الايقاف للبروتونات وجسيمة الفا في البولي كاربونيت (PC) $C_{16}H_{14}O_3$والبولي يورثين (PU)$C_{27}H_{36}N_2O_{10}$

الخلاصة:

في هذا البحث تم حساب قدرة الايقاف للجسيمات المشحونة باستخدام معادلات Betheو Bragg وZiegler للبروتونات وجسيمة الفا في بولي كاربونيت $C_{16}H_{14}O_3$ و بولي يورثين $C_{27}H_{36}N_2O_{10}$ في مدى طاقه MeV(0.01-1000). تم برمجة المعادلات باستخدام MATLAB 2021، وتمت مقارنة الحسابات مع البيانات التجريبية لبرنامج P-STAR وSRIM 2013 و A-STAR، واظهرت هذه المقارنة توافقاً جيداً مع البيانات التجريبية في منطقة الطاقة المتوسطة و العالية بالنسبة لمعادلة بيث. كما اظهرت النتائج ان قدرة الايقاف المحسوبة طبقاً لمعادلات زيكلر تتوافق بشكل جيد مع البيانات التجريبية في جميع مديات الطاقة وكان معامل الارتباط (0.9) تم اختيار هذه الاهداف لاهميتها في المجالات الصناعية والكيميائية.

الكلمات المفتاحية: قدرة الايقاف،P-star، A-star،Srim2013،بيث ،زيكلر ،قاعدة براغ.