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Research Article

Calculation Of Stopping Power Of Protons And Alpha Particles In PMMA, $C_5O_2H_8$, And PAA, $C_3O_2H_4$

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ABSTRACT

In this research, the stopping power of charged particles was calculated using the Bethe, Bragg and Ziegler equations for protons and the alpha particle in polymethylmethacrylate $C_5O_2H_8$ and polyacrylic acid $C_3O_2H_4$ in the MeV energy range (0.01-1000). The Bethe, Bragg and Ziegler equations were used and the equations were programmed using MATLAB 2021. The calculations were compared with the imperical data of the P-STAR, SRIM 2013 and A-STAR programs. This comparison showed good compatibility with the imperical data in the medium and high energy region for the Bethe equation. The results also showed that the stopping power calculated according to the Ziegler equations corresponds well with imperical data in all energy ranges. The correlation coefficient was (0.9). These targets were chosen for their importance in the industrial and chemical fields.

Key Words : stopping power, P-star, A-star, Srim2013, Bethe's equation, Ziegler's equations, Bragg rule

1. Introduction

The penetration of charged particles of matter has aroused interest since early modern atomic physics. One of the important and main topics in this field is the energy transferred from the projectile to the atomic target. The first to study this theory was Niels Bohr, who developed its theoretical framework based on classical mechanics, followed by others who followed the method of classical mechanics and quantum mechanics to show that the phenomenon of association with this field is the energy transferred from shells to the atom .There are many theoretical models that are limited to many hypotheses or using simple ideas that have no applications in real physical systems, and experimental measurements of the energy loss of passing particles have an important role in understanding these interactions. The loss of energy for the unit of distance in the target material is called (Stopping power) and is expressed in the form of -dE/dx and is expressed in units MeV.cm^{-1}, which depends on the charge of the projectile as well as the material of the target [1]. Bethe theory is valid only at high velocity and collapses at low velocity because the basis of Bethe theory comes from the calculation of the first degree of turbulence theory based on the condition Bethe's equation is $\left(K_B = \frac{2Z_1V_0}{V}\right)$ applied, that is, the magnitude is high in it, so the Bethe theory cannot (Z_1/V) be used for very heavy falling particles such as fission fragments due to high atomic charge and low velocity [2], and the Bethe theory is also valid when the velocity of the falling particle is higher than the velocity of Bohr [3].
The aim of this research is to study the stopping capacity to collect information about the proton shell and the alpha particle in polymers $(C_5O_2H_8, C_3H_4O_2)$ using the Bethe, Bragg and Ziegler equations.

2. My theory

Heavy charged particles travel in a straight path through matter. As these particles continue to move, energy will be transferred continuously to the electrons of the physical medium. When the particles slow down, the kinetic energy is reduced and converted into thermal energy in the atoms of the physical medium. The interaction of heavy charged particles with matter leads to a flexible collision with the nucleus of the target atom. The energy that is transferred as a result of flexible and inelastic collisions to the nucleus is neglected and not taken into account [4, 5]. Stopping power can be defined as a common term for the loss of energy caused by all electronic processes, as the energy of the moving particles in the material of the atomic mass unit is greater than (1 keV/ amu) for the loss of kinetic energy by means of the electronic stopping power [6]. The electronic stopping power has been studied theoretically and experimentally since the beginning of the twentieth century, especially for heavy ions for their important role in nuclear and atomic physics[7]. The stopping power is calculated according to classical mechanics according to Bohr's theory (Bohr, 1913) and according to quantum mechanics according to Bethe's theory (Bethe, 1930). The stopping power is calculated by linking classical and quantum mechanics with the Kappa coefficient (K_B) that distinguishes classical dispersion from quantum disorder [8].

The ability to stop is given by the following equation:

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

where:

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

S_i: the stopping power of the element and W_i: the weight ratio of the element in the compound and N_i: the number of atoms in the compound and A_i: the atomic mass of the medium and Bethe's equation is written as follows:

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

K_o *: equals* (K_0=8.99×10⁹ N.$m^2\backslash c^2$), m_e: Equal to (9.1×10^{-31} kg), mc^2: Static energy of the electron equal to (5.11×10^5 eV), Z_1: Atomic number of the proton (Z_1=1), Z_1: Atomic number of alpha particles (Z_2=2), e: Electron charge (1.6× 10^{-19} C), c:Speed of light in space equal to (3x10^8 m/sec), N_A: Avcadro number equal to (6.023×10^{23} mol), β: Relative speed equal to ($\beta = v/c$), and I:Average ionization voltage (eV) where:

$$\beta^2 = 1 - \frac{1}{(1 + \mathrm{Ep}\backslash 931.5\, M_1)^2} \quad (4)$$

M_1: for a proton is equal to (1.008) and M_1: for an alpha particle is equal to (4.002) in the unit of atomic masses. The ionization voltage is defined as the minimum amount of energy that must be given to one linked electron sufficient to transfer it from its orbit. Electrons in external orbits for ionization are less than electrons in internal orbits. As a result, they need high energy to ionize electrons in external orbits. As a result, the rate of ionization voltage is considered an important coefficient in theoretical stopping power calculations because it depends on the electronic arrangement of atoms and molecules in the stopping medium and their physical state [9]. Therefore, many atomic properties depend on the ionization effort, such as the cross section of the stopping and its ability to stop and polarize. Researchers have resorted to measuring the ionization potential practically because it is difficult to calculate it theoretically by analyzing the stopping capacity of high-energy protons [10]. The ionization effort is given by the following relationships:

$$I = \begin{cases} 19.2 & eV \quad if\ Z_2 = 1 \\ 11.2 + 11.7 & eV \quad if\ 2 \le Z_2 \le 13 \\ 52.8 + 8.71 Z_2 & eV \quad if\ Z_2 > 13 \end{cases} \quad (5)$$

The Ziegler equations for the proton have also been adopted and are written as follows:

2.1- Electronic stopping power equations:

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

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

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

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

where:

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

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

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 Suspension Capacity 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:*

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

where*:*

$$\varepsilon = \frac{32.53M_2E}{Z_1Z_2(M_1+M_2)(Z_1^{0.23}+Z_2^{0.23})} \quad (13)$$

The Ziegler equations for the alpha particle are written as follows:

1- Nuclear stopping power equations:

$$\varepsilon = \frac{32.53M_2E}{Z_1Z_2(M_1+M_2)\left(Z_1^{\frac{2}{3}}+Z_2^{\frac{2}{3}}\right)^{1/2}} \qquad (14)$$

If (ε< 0.01) the equation used:

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

When the energy is (0.01 ≤ ε ≤ 10) the equation used:

$$S_{nz} = 1.7(\varepsilon^{1/2})\left[\ln(\varepsilon+exp1)/1+6.8\varepsilon+3.4\varepsilon^{3/2}\right] \qquad (16)$$

If (ε > 10)the equation used:

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

2-Electronic stopping power equations:

If the energy (E≤ 10^4):

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

where:

$$S_{low} = A_1E^{A2} \quad (19)$$

$$S_{high} = \frac{1000A_3}{E}\ln\left(1+\frac{1000A_4}{E}+\frac{A_5E}{1000}\right) \quad (20)$$

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

$$S_{ez} = \exp\left(A_6+A_7\ln\left(\frac{1000}{E}\right)+A_8\ln\left(\frac{1000}{E}\right)^2+A_9ln\left(\frac{1000}{E}\right)^3\right) \quad (21)$$

3. Results and discussion

Table (1) shows the results of the stopping power of the protons that were used in the polymers ($C_5O_2H_8, C_3H_4O_2$). Table No. (2) shows the results of the stopping power of alpha particles in polymers ($C_5O_2H_8, C_3H_4O_2$).

Table 1: Calculations of the stopping power of the proton in polymethyl methacrylate and polyacrylic acid

E_{proton}	PMMA				PAA			
Energy = MeV	Bethe	Zeigler	P-Star	SRIM	Bethe	Zeigler	P-Star	SRIM
0.01	-9134.93	546.56	539.18	504.64	-9638.35	485.59	479.51	441.79
0.1	869.39	923.70	918.35	883.67	779.20	845.38	840.88	807.17
1	265.52	267.65	259.41	254.35	252.50	257.37	247.08	240.86
10	44.94	45.98	45.12	45.53	43.21	44.57	43.46	43.82
50	12.16	12.45	12.24	12.31	11.73	12.10	11.84	11.90
100	7.11	7.27	7.16	7.19	6.87	7.06	6.93	6.96

150	5.31	5.42	5.34	5.37	5.13	5.27	5.17	5.19
200	4.38	4.46	4.40	4.42	4.23	4.34	4.27	4.28
225	4.06	4.14	4.09	4.10	3.93	4.03	3.96	3.97
250	3.81	3.88	3.83	3.85	3.69	3.78	3.71	3.73
275	3.60	3.67	3.62	3.64	3.49	3.57	3.51	3.52
300	3.43	3.49	3.45	3.46	3.32	3.40	3.34	3.35
350	3.16	3.21	3.17	3.18	3.05	3.13	3.07	3.08
400	2.95	3.01	2.96	2.98	2.86	2.92	2.87	2.88
450	2.80	2.84	2.80	2.82	2.71	2.77	2.72	2.73
500	2.67	2.72	2.68	2.69	2.59	2.64	2.60	2.61
550	2.57	2.61	2.58	2.58	2.49	2.54	2.50	2.51
600	2.49	2.53	2.49	2.50	2.41	2.46	2.42	2.42
650	2.42	2.46	2.42	2.43	2.34	2.39	2.35	2.36
700	2.36	2.40	2.36	2.37	2.29	2.34	2.29	2.30
800	2.27	2.31	2.27	2.28	2.20	2.25	2.20	2.21
900	2.20	2.24	2.20	2.21	2.13	2.18	2.13	2.14
1000	2.15	2.19	2.15	2.15	2.09	2.13	2.08	2.09

Table 2: **Stopping power calculations for alpha particle in polymethyl methacrylate and polyacrylic acid**

Alpha Lep Energy = MeV	**PMMA**				**PAA**			
	Bethe	**Zeigler**	**A-star**	**SRIM**	**Bethe**	**Zeigler**	**A-star**	**SRIM**
0.01	-314613	508.31	563.05	516.73	-318819	446.91	521.81	472.57
0.1	-3148.52	1287.94	1399.32	1310.57	-4201.85	1163.12	1289.04	1199.95
1	2517.05	1994.61	2223.78	2145.82	2348.40	1883.09	2089.46	2005.44
10	536.44	536.79	530.81	549.96	513.18	513.17	508.43	525.30
50	149.00	155.36	149.76	151.82	143.38	148.33	144.35	146.25
100	84.61	89.21	85.20	86.08	81.55	85.06	82.26	83.06
150	60.88	64.77	61.34	61.87	58.72	61.68	59.26	59.75
200	48.34	51.82	48.70	49.10	46.65	49.29	47.08	47.43
225	44.03	47.36	44.37	44.71	42.50	45.03	42.90	43.20
250	40.53	43.73	40.83	41.14	39.13	41.55	39.48	39.76
275	37.62	40.71	37.91	38.18	36.33	38.67	36.66	36.91
300	35.17	38.16	35.44	35.69	33.97	36.23	34.28	34.50
350	31.26	34.07	31.50	31.71	30.20	32.32	30.47	30.66
400	28.28	30.93	28.49	28.68	27.32	29.32	27.57	27.73
450	25.93	28.45	26.11	26.28	25.05	26.95	25.27	25.42
500	24.02	26.42	24.19	24.34	23.21	25.01	23.42	23.55
550	22.45	24.74	22.61	22.74	21.70	23.40	21.88	22.00
600	21.12	23.31	21.27	21.39	20.42	22.04	20.59	20.70
650	20.00	22.09	20.13	20.24	19.33	20.88	19.49	19.59
700	19.02	21.03	19.15	19.25	18.39	19.87	18.55	18.63
800	17.43	19.28	17.54	17.63	16.85	18.19	16.99	17.07
900	16.18	17.88	16.28	16.36	15.65	16.86	15.77	15.84
1000	15.18	16.75	15.26	15.34	14.68	15.78	14.79	14.85

The stopping power of the protons of the two polymers ($\mathbf{C_3H_4O_2}$,$\mathbf{C_5O_2H_8}$) was calculated within the energy (0.01-1000 MeV). Which was calculated by the Bethe and Zeigler equations and applied to the elements (C, H, O, N) individually and then we applied the Bragg equation to the polymer and all the mentioned equations were programmed using MATLAB 2021. Figures (1, 3) show the comparison between the theoretically calculated results of the stopping power values as a function of the proton energy of the above equations with the calculated results of the SREM 2013 program and the results of the P-STAR using the MATLAB 2021 program .When applying the Bethe equation, we notice that it gives negative values for the stopping power at low energies, where we note the cut off in Figure (1), which is within the energies (0.01 <E< 0.03 MeV) in Figure (3), the cut off limit is within the energies (0.01 <E< 0.035 MeV). This is because it does not have a physical reality, and the reason for the negative value is the logarithm. Its meaning is the shell. Everything that enters the material instead of its speed increases, and this is contrary to reality. A cutoff process is carried out because of the logarithm in the Bethe equation, so the cutoff for these negative results is at these energies . The validity of Bethe's theory also depends on the hypothesis that the velocity of the falling particle is much greater than the motion of the orbital electrons of the atoms of the target material.
The greatest stopping power value for protons was observed when applying the Bethe equation in Figure (1). It is at energy E=0.09 MeV. In Figure (3), the greatest stopping power value is at energy E=0.1 MeV. The greatest stopping power is due to the ionization and extraction of atoms. After these maximum stopping power values, the stopping power decreases as the energy of the falling particle increases. The reason for this rapid decrease when applying the Bethe equation is due to the fact that the energy is inversely proportional to the square of the velocity of the falling particle ($1\backslash \boldsymbol{v}^2$) or vice versa with the energy of the projectile. At these energies, electronic deactivation is predominant. We note that the results of the Bethe equation are far from the experimental values of the SREM 2013 program and the P-STAR program in low energies and are consistent with these experimental values of the two programs when the energy is high because the Bethe equation is quantitative and suitable for high energies.
Using the equations developed by Ziegler to calculate the stopping power of protons , where the energy zones were divided into three zones : in the low-energy zone (E <10 MeV)), we note in Figures (1,3) that the values of the stopping power are low with a slow increase due to the low speed of the particle, as nuclear collisions in this region are prevalent .As for the medium energy area (10<E<100 MeV), we note through Figures (1,3) that the stopping power has clearly increased and reaches its greatest stopping power due to the ionization and excitation of the atoms of the material in this area. In Figure (1), the stopping power is at its greatest amount at energy E=0.08 MeV. In Figure (3), the stopping power is at its greatest amount at energy E=0.2 MeV, which are results that correspond well with the results of SREM 2013and the results of P-STAR. As for the high energy areas, (100<E<1000 MeV), we note from Figures (1,3) that after the stopping power reaches its peak in the medium energy area, it gradually begins to decrease and continues to increase the falling particle, because the loss of energy is inversely proportional to the square of the particle's velocity, and then the electronic stopping is prevalent. The correlation coefficient Rc was calculated based on the stopping power values calculated from Beth's equations, Zucker's equations, and SREM2013 data. The P-STAR values for Figure (1) were P-star vs Bethe_p and its value was (0.9547) and its value between Zeigler_p vs SRIM_p is (0.9998) and for Figure (3) was between P-star vs Bethe_p and its value was (0.9578) and between Zeigler_p vs SRIM_p and its value was (0.9998).
We calculate the stopping power of alpha particles of polymerine ($\mathbf{C_3H_4O_2}$, $\mathbf{C_5O_2H_8}$) within the energy (0.01-1000 MeV).Which was calculated by the Bethe and Zeigler equations and applied to the elements (C,H,O,N) individually and then we applied the Prague equation to the polymer and all the mentioned equations were programmed using MATLAB 2021. Figures (2, 4) show the comparison between the theoretically calculated results of the stopping power values as a function of the energy of alpha particles from the above equations with the calculated results of the SREM 2013 program and the results of A-STAR using the MATLAB 2021 program .When applying the Bethe equation, we notice that it gives negative values for the ability to stop at low energies, as we note that the cut off limit in Figure (2) is within the energies of (0.01<E<0.1 MeV). In Figure (4), the cut-off limit is within the energies of (0.01<E<0.03 MeV). This is because it does not have a physical reality and the reason for the negative value is the logarithmic meaning of the shell. Everything that enters the material instead of its speed decreases increases, and this is contrary to reality. A cut-off process is carried out because of the logarithm in the Bethe equation, so the cut-off for these negative results is at these energies. The validity of Beth's theory also depends on the hypothesis that the velocity of the falling particle is much greater than the motion of the orbital electrons of the atoms of the target material.
We note that the greatest stopping power value for alpha particles when applying the Bethe equation in Figure (2) is at energy E=0.35 MeV , while in Figure (4) the greatest stopping power value is at energy E=0.4 MeV , and that the greatest stopping power is due to the ionization and irritation of the atoms, then after these maximum stopping power values decrease with the increase in the energy of the falling particle, and that the reason for this rapid decrease when applying the Bethe equation is due to the fact that the energy is inversely proportional to the square of the velocity of the falling particle ($1\backslash \boldsymbol{v}^2$) or vice versa with the energy of the projectile . At these energies, electronic deactivation is predominant. We note that the results of the Bethe equation are far from the experimental values of the SREM2013 program and the A-STAR program in low energies and are consistent with these experimental values of the two programs when the energy is high because the Bethe equation is quantitative and suitable for high energies.

Using the equations developed by Ziegler to calculate the stopping power of alpha particles, we note from Figure (2) that the stopping power of alpha particles using the Ziegler equations is the greatest amount at energy E=0.9 MeV, while in Figure (4) the stopping power is the greatest amount at E=0.7 MeV, which are good results that correspond to the practical statements of the SREM 2013 program and the practical statements of theA-STAR program. The correlation coefficient Rc was calculated based on the stopping power values calculated from Bethe's equations, Ziegler's equations, SREM 2013 data, and A-STAR's values. The stopping power of Figure (2) was between A-star vs Bethe and its value (0.9621), and its value in Figure (4) was between Zeigler vs SRIM (0.9993).

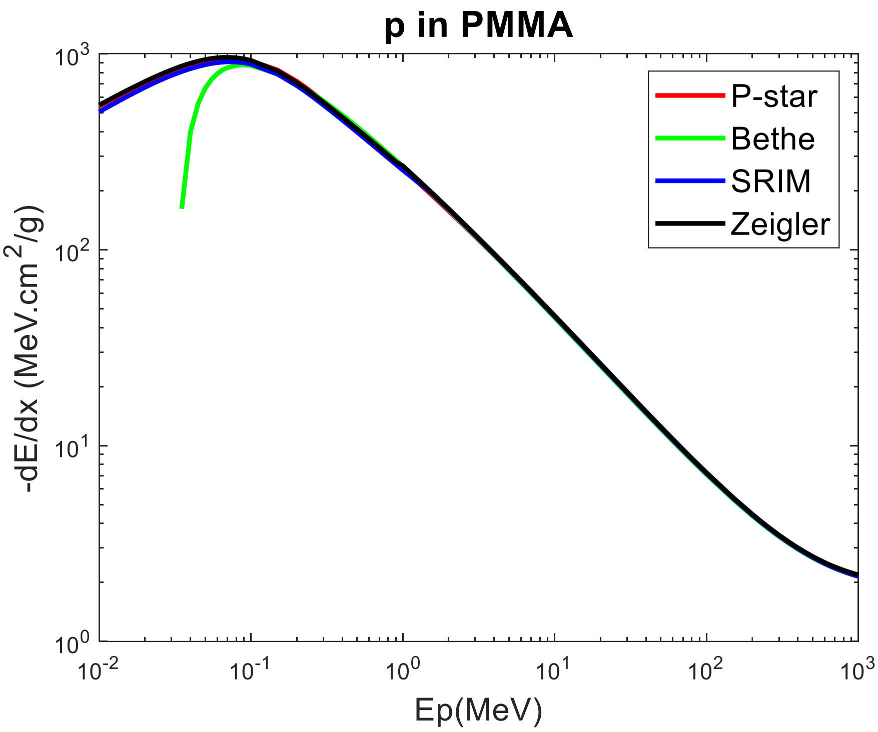

Figure 1: Proton stopping power in polymethyl methacrylate

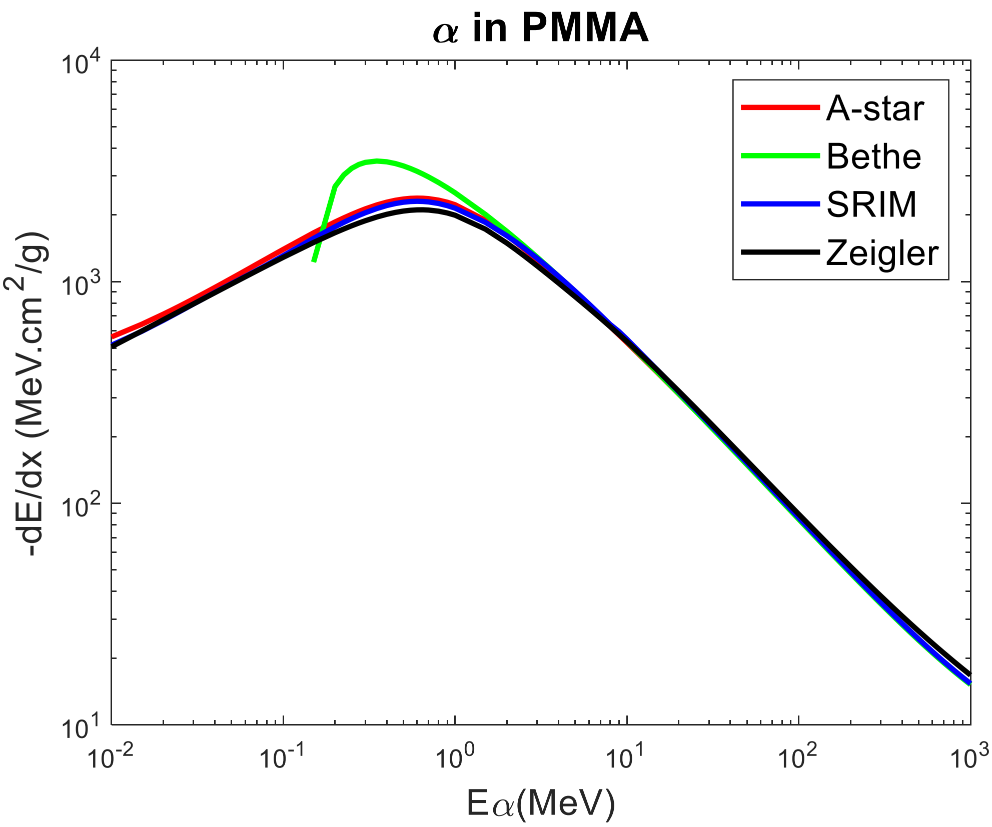

Figure 2: Stopping power of alpha particle in a polymethyl methacrylate.

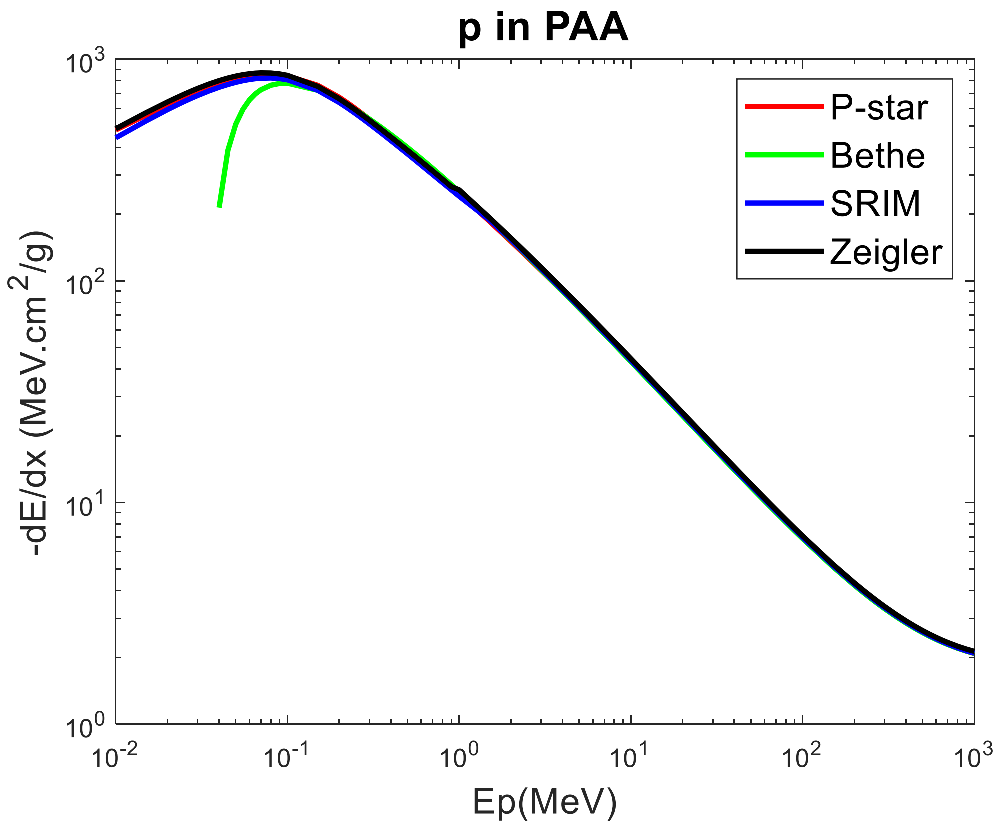

Figure 3: Proton stopping power in polyacrylic acid.

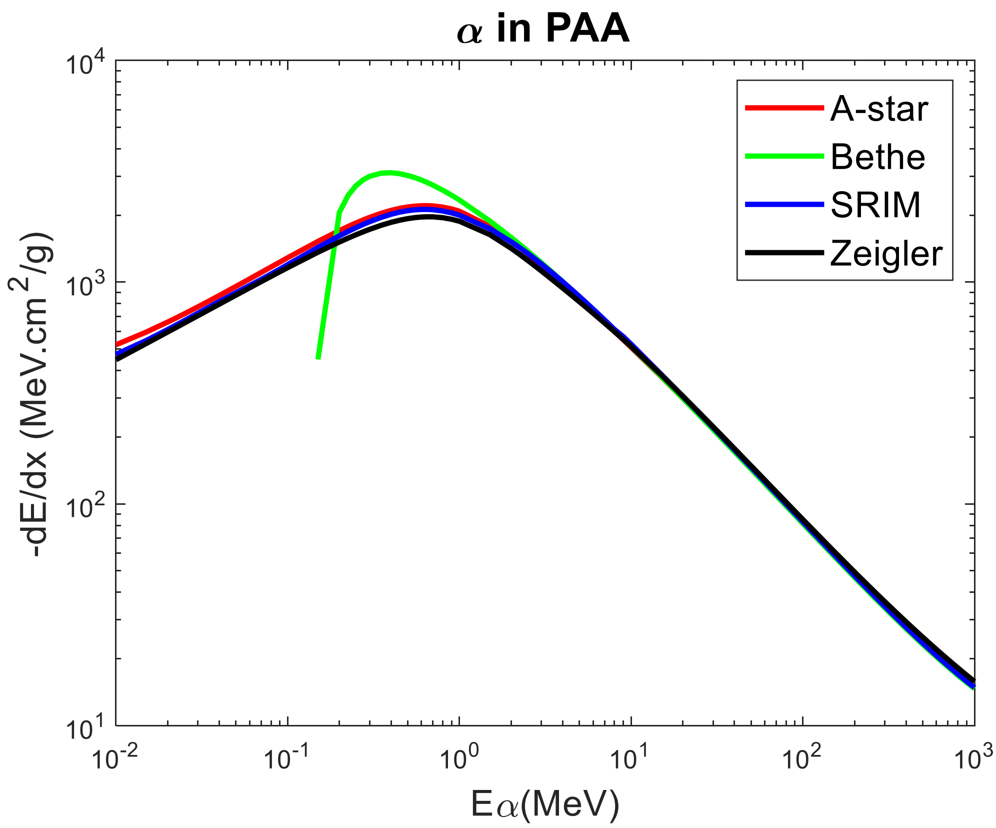

Figure 4: Alpha particle stopping power in polyacrylic acid

4. Conclusions

From the results obtained from this study, we conclude the following:

1- The stopping power calculated according to *Ziegler* 's equations corresponds well with experimental data in all power ranges.

2- This comparison showed good compatibility with experimental data in the medium and high energy region for the Bethe equation.

3- We found that the greatest stopping power value for PMMA according to the Bethe equation is greater than the greatest stopping power value according to the Ziegler equation for protons, while we found the greatest stopping power value according to the Bethe equation is less than the greatest stopping power value according to the Ziegler equation for alpha particles.

4- We found that the greatest stopping power value for protons in a PAA polymer according to the Bethe equation is greater than the greatest stopping power value according to the Ziegler equation for protons, while we found the greatest stopping power value according to the Bethe equation is less than the greatest stopping power value according to the Ziegler equation for alpha particles.

5- The stopping power of the PMMA polymer reaches its maximum amount at the energies of (0.01-0.09 MeV) for protons, and at the energies range of (0.01-0.35 MeV) for alpha particles according to the Beth equation for the studied compounds, and then it begins to decrease gradually with the increase of the energy of the projectile.

6- The stopping power of the PAA polymer reaches its maximum amount at the energies of (0.01-0.1 MeV) for protons, and at the energies range of (0.01-0.4 MeV) for alpha particles according to the Bethe equation for the studied compounds and then gradually decreases as the energy of the projectile increases.

7- The stopping power in two polymers reaches its maximum amount at the energies of (0.01-0.07 MeV) for protons, and at the energies of (0.01-0.65 MeV) for alpha particles according to the Ziegler equation for the studied compounds, and then it begins to decrease gradually with the increase in the energy of the projectile.

8- Through the results, we note that the value of the stopping power according to Bethe when the proton energy is 0.01MeV is negative and the amount of 9134.93 MeV for the polymer, the value of the stopping power Bethe when the particle energy of Alpha is 0.01 MeV is negative and the amount of 9638.35 MeV for the polymer.Through the results, it is noted that the stopping power at energy 0.01MeV is negative, and we conclude that the Beth equation is invalid at energies $E \leq 0.01$MeV

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