Journal of Engineering and Applied Sciences 13 (23): 9898-9902, 2018
ISSN: 1816-949X

Total Stopping Power Calculations of C_2H_4O, C_3H_6 and C_3H_3N for Electrons

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Abstract: In this research, the values of radiative stopping power (S_{rad}), collisional stopping power (S_{coll}) the total stopping power and stopping time for electrons in C_2H_4O, C_3H_6, C_3H_3N adopted Bethe-Bloch relativistic formula in the energy range of 0.01-1000 MeV have been studied. The results were showing the radiative stopping power dominate more than the collisional stopping power in the total stopping power which are in good agreement with estar universal code results.

Key words: Theoretical Physics, Bethe-Bloch, stopping power, stopping time, radiative, collision, mean excitation energy, C_2H_4O, C_3H_6, C_3H_3N, estar code

INTRODUCTION

When charged particles pass through the material. It will lose their energy due to their interaction with target atoms. The energy loss of the projectile per unit distance in the target material is called the stopping power of the material and is usually written as -dE/dX (Chandrasekharan and Gupta, 2006).

When the incident electron collides with the atom, it is probably that the following interaction interact may be happen: the incident electron scattered elastically and leaves the atom without any perturbation, the incident electron scattered in elastically and excites the atom then transfers the orbital electrons from a low energy level to a high energy level, the incident electron ionizes the atom by uprooting one of its orbiting electrons, the incident electron scattered from nuclei it emits a Bremsstrahlung photons. The stopping power of electrons in a media. The knowledge of such physical quantities are very important in the electron radiotherapy and in the calculation of radiation dose. Electron can emit electromagnetic radiation which is known as Bremsstrahlung photons. The energy loss due to ionization and excitation is known as collisional energy loss (Berger and Seltzer, 1964; Agrawal *et al*., 2011). The calculation of energy loss due to emission of Bremsstrahlung is more complicated than the calculation of energy loss due to ionization and excitation and there is no exact formula used in such calculations but there are only an approximate equations (Mayles *et al*., 2007; Attix, 1986) that will be given for the calculation of radiative loss for electrons only, since, the energy loss by Bremsstrahlung radiation is important which is less importance for heavy charged particles (Al-Ajili *et al*., 2016).

MATERIALS AND METHODS

Theory: The collisional stopping power (S_{coll}) is defined as hard collision with atomic electrons, the electron loses its energy by ionization and excitation the orbital electrons of the absorbent medium. stopping power (dE/dX) can be defined as the rate of energy loss per unit path length of an electron or positron by excitation and ionization which was known as "collisional energy loss". The collisional stopping power for electrons is given by (Berger and Seltzer, 1983; Gumus *et al*., 2006):

$$\left(\frac{-dE}{dX}\right)_{coll} = \frac{2\pi r_e^2 m_e c^2 Z N_A}{\beta^2 A}\ln\frac{E^2}{I} + \ln\left(1+\frac{\tau}{2}\right) + F^-(\tau) - \delta \quad (1)$$

Where:

r_e = Classical electron radius $e^2/m_ec^2 = 2.818*10^{-15}$ m
m_e = The rest mass of electron = $9.11*10^{-31}$ kg
c = The speed of light in the vacuum = $3*10^8$ m/sec
v = The speed of light in the target material
m_ec^2 = Rest mass energy of the electron = 0.511 MeV
Z = Atomic number of target material
N_A = Avogadro's Number = $6.022*10^{23}$ atoms/mole
A = Atomic mass of medium
β = A correction factor. $\beta = v/c$
I = The Ionization potential of the medium (eV)
δ = Density effect correction to electronic energy loss
E = The Energy of the incident electron
τ = The kinetic energy of electron in terms rest energy

$$\tau = \frac{E}{m_ec^2} \quad F^-(\tau) = \left(1-\beta^2\right) + 1 + \frac{\tau^2}{8}(2\tau+1)\ln 2 \quad (2)$$

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Table 1: Equation constants (Eq. 3) $\overline{X_0}$, $\overline{X_1}$, $\overline{C}$, $\overline{a}$, and $\overline{m}$ (Sternheimer *et al.*, 1984)

Target	$\overline{C}$	$\overline{X}_o$	$\overline{X}_1$	$\overline{a}$	$\overline{m}$
C_2H_4O	-3.1115	0.1401	2.6315	0.11178	3.3893
C_3H_6	-3.1252	0.1534	2.4822	0.15045	3.2855
C_3H_3N	-3.2459	0.1504	2.5159	0.16275	3.1975

δ is the polarization or density effect correction in condensed medium (Berger and Seltzer, 1983; Sternheimer *et al.*, 1982):

$$\left.\begin{aligned} &\delta = 0 && \overline{X}<\overline{X}_o \\ &\delta = (4.606\times\overline{X})+\overline{C}+[\overline{a}(\overline{X}_1-\overline{X})^{\overline{m}}]\overline{X}_o<\overline{X}<\overline{X}_1 \\ &\delta = (4.606\times\overline{X})+\overline{C}\;\overline{X}>\overline{X}_1 \end{aligned}\right\} \quad (3)$$

Where:

$$\overline{X} = \log\left(\log\left(\frac{\beta}{\sqrt{1-\beta^2}}\right)\right) \quad (4)$$

The constants of Eq. 3 are shown in Table 1

Radiative stopping power: Bremsstrahlung emitted from the collision of heavy charged particles with an atom can be ignored because of heavy particles are not accelerated. On the other hand, electrons receive strong acceleration and emit bremsstrahlung. The definition of mass radiative stopping power is given by the bremsstrahlung efficiency is proportion to Z^2 and linearly increases depending on electron energy. The collision stopping power for high-energy electrons show the logarithmic increase. Bremsstrahlung becomes a dominant mechanism of energy loss at high energies. The next approximation is the ratio between collisional stopping power and radioactive stopping power by Nikjoo *et al.* (2012) and Bethe (1932):

$$\frac{S_{rad}}{S_{coll}} \cong \frac{E\,Z}{800} \quad (5)$$

Where:

Z = The atomic number of the target atom and
E = The energy of the incident electron in MeV

$$S_{tot} = S_{rad}+S_{coll} \quad (6)$$

Through compensation Eq. 5 in Eq. 6 we get (Pal *et al.*, 1986):

$$S_{tot} = S_{coll}\left(1+\frac{E\,Z}{800}\right) \quad (7)$$

The mean ionization potential I: The mean ionization potential I(eV) defined as the geometric mean value of all ionizations and excitation potentials of an atom in the absorbing medium. The formula of the mean ionization potential (I) (Bloch, 1933; Dalton and Turner, 1968). For elements:

$$\left.\begin{aligned} &I = 19(eV)\;Z = 1 \\ &I = 11.20+11.7Z \quad (eV)\;2\le Z\le 13 \\ &I = 52.8+8.71Z \quad (eV) \quad Z>13 \end{aligned}\right\} \quad (8)$$

For a compound (Podgorsak, 2013):

$$I = \exp\left(\frac{\sum(N_i\times Z_i\times \ln I_i)}{n}\right) \quad (9)$$

Where:

N_i = Atoms cm^{-3} for ith element with Z_i and I_i
$n = \sum N_i Z_i$ = Total number of electrons in the mixture

Stopping time: The stopping time is the time interval required to stop a charge particle in an absorber medium. This time can be expressed in terms of the stopping power by using the chain of differentiation (Ahmed, 2007).

$$\frac{dE}{dt} = \left(\frac{dE}{\rho dx}\right)\left(\frac{\rho dx}{dt}\right) = \frac{1}{\rho}\left(\frac{dE}{dx}\right)(\rho v) = \rho v\left(\frac{dE}{\rho dx}\right) \quad (10)$$

where, v = dx/dt is the velocity of the particle. A rough estimate can be made of the time it takes a heavy charged particle to stop in matter, if one assumes that the slowing-down rate is constant. For a particle with kinetic energy E, this time is approximately (Turner, 2008).

$$t = \frac{E}{dE/dt} = \frac{E}{\rho v(de/\rho dx)} \quad (11)$$

where, t in unit (sec)

RESULTS AND DISCUSSION

The results of S_{tot} are illustrated in Fig 1-3 shows these results are obtained by application the Eq. 1-6 which had been written by the language of the MATLAB 2016 for C_2H_4O, C_3H_3N and C_3H_6 in the energy range (0.01-1000) MeV. Figure 1-3 showed a good agreement with estar code and correlation coefficient (r = 0.99). When the electron entered a material, it's not only lost the kinetic energy only but its directional changes continuously and this particles suffering from many deviations at large angles along its path length after approaches the nuclear field of target atom . The nature of collisional interactions of incident electrons and orbital electrons resulting from the interactions of the electrical

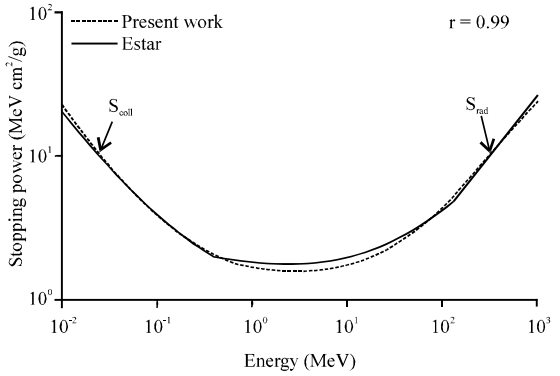

Fig. 1: Comparison of the present work and estar results for the total stopping power of C_3H_3N as a function of projectile energy for electrons

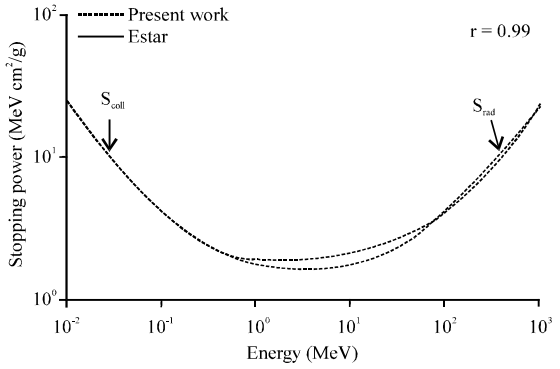

Fig. 2: Comparison of the present work and estar results for the total stopping power of C_3H_6 as a function of projectile energy for electrons

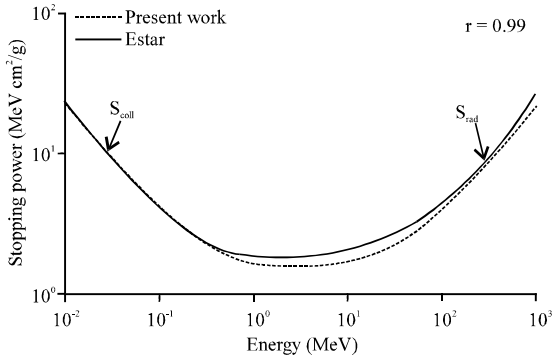

Fig. 3: Comparison of the present work and estar results for the total stopping power of C_2H_4O as a function of projectile energy for electrons

fields of both electrons, the incident electron as approaches the orbital electrons not an actual contact occurs between them, the S_{rad} values proportional to the incident electron energy E and this situation can be

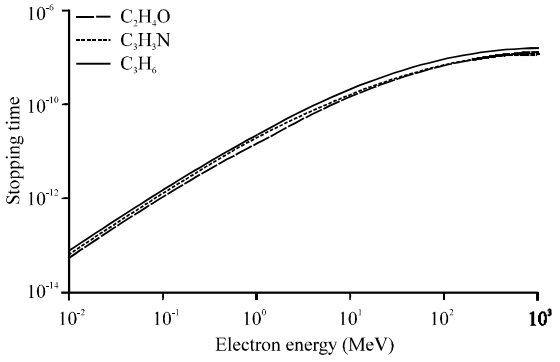

Fig. 4: Calculated stopping time of polymers (C_2H_4O, C_3H_3N, C_3H_6) for electrons

explained that the slow electrons (low energy electron) spend most its time in interactions with orbital electrons and this indicates that these electron has high probability of interactions with atomic electrons while the fast electrons has low probability of interactions with these electron and pass over the columbic field without influenced by the electrons, thus, this induced the electrons to open more channels of radiative energy losses. When we compare the results of both S_{coll} and S_{rad}, we found that, the S_{coll} dominates over the S_{rad} due to the low energy range and the most contribution in S_{tot} is due to it. Figure 1-3, we observed a divergence of present results and estar, at energy range (2-60) MeV, this difference was due to two reasons, first reason the values of S_{rad} in estar were calculated by Berger-Seltzer equation while present results was calculated by equation $S_{rad} = S_{coll}$ (EZ/800) the second reason in this region there is a state of stability of the tow stopping powers (S_{rad} and S_{coll}), so that, the bottom of the point is that S_{tot} is less than possible. Figure 4 shows the stopping time is proportional to the energy of electrons according to the equations the multi boundary is that:

{for C_2H_4O curve fit is: $y = -0.136388182 x^2 + 1.038804963x - 10.74717607$}

{for C_3H_3N curve fit is: $y = -0.140592675 x^2 + 1.026391366x - 10.69517729$}

{for C_3H_6 curve fit is: $y = -0.137711319x^2 + 1.039059353x - 10.61864828$}

where, y = log t and x = log T. It also, appears that the time of the electrons in mediums (C_2H_4O, C_3H_3N and C_3H_6) has value highest in energies >100 MeV and increase at idle time there is little power increase for electrons. Figure 5-7 shows the change density effect correction for estar and present results

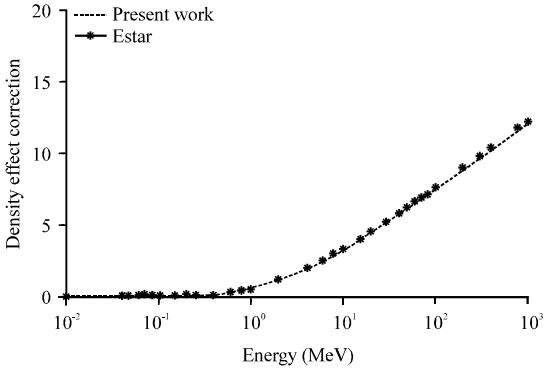

Fig. 5: Comparison of the present work and estar results for the density effect correction of C_2H_4O for electrons

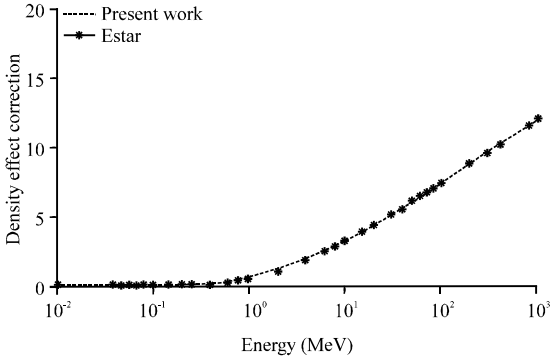

Fig. 6: Comparison of the present work and to be results for density effect correction of C_3H_3N for electrons

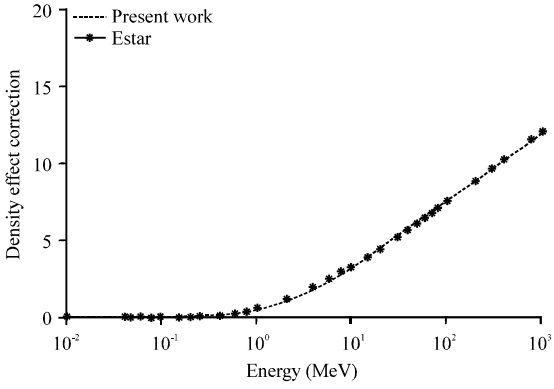

Fig. 7: Comparison of the present work and estar results for density effect correction of C_3H_6 for electrons

with electrons energy it shows that the density effect correction values begin its effect after energies >1 MeV where the density effect correction increase with increase electrons energy which are in good agreement with estar. Figure 8 show the change density effect correction with electrons energy in mediums (C_2H_4O, C_3H_3N and C_3H_6).

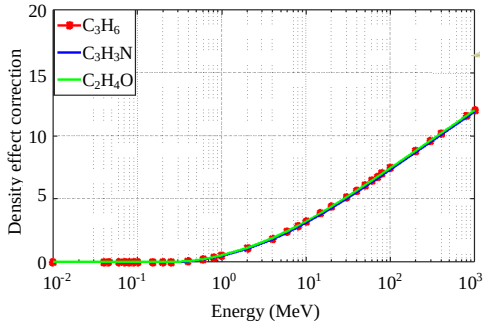

Fig. 8: Calculated density effect correction of (C_3H_6 ,C_3H_3N ,C_2H_4O) for electrons

Table 2: Density effect correction of C_2H_4O, C_3H_3N and C_3H_6 for electrons as well as the parameter X

E (MeV)	X	δ C_2H_4O	δ C_3H_3N	δ C_3H_6
0.01	-0.7020	0	0	0
0.04	-0.3947	0	0	0
0.045	-0.3681	0	0	0
0.06	-0.3026	0	0	0
0.07	-0.2672	0	0	0
0.08	-0.2362	0	0	0
0.09	-0.2086	0	0	0
0.1	-0.1838	0	0	0
0.15	-0.0863	0	0	0
0.2	-0.0148	0	0	0
0.25	0.0423	0	0	0
0.4	0.1686	0.0369	0.0219	0.0187
0.6	0.2852	0.2144	0.1844	0.1858
0.8	0.3729	0.3746	0.3335	0.3395
1	0.4439	0.5203	0.4705	0.4808
2	0.6816	1.1028	1.0259	1.0532
4	0.9424	1.8898	1.7882	1.8367
6	1.1032	2.4405	2.3267	2.3886
8	1.2201	2.8676	2.7465	2.8177
10	1.3120	3.2176	3.0918	3.1700
15	1.4813	3.8908	3.7583	3.8484
20	1.6027	4.3936	4.2579	4.3555
30	1.7752	5.1313	4.9932	5.0997
40	1.8984	5.6715	5.5329	5.6444
50	1.9942	6.0981	5.9597	6.0744
60	2.0727	6.4507	6.3128	6.4295
70	2.1391	6.7513	6.6139	6.7319
80	2.1967	7.0131	6.8763	6.9952
100	2.2930	7.4531	7.3172	7.4372
200	2.5930	8.8317	8.6973	8.8180
300	2.7687	9.6411	9.5067	9.6274
400	2.8935	10.2157	10.0813	10.2020
800	3.1942	11.6010	11.4666	11.5873
1000	3.2911	12.0471	11.9127	12.0334

Table 1 shows equation constants for density effect correction $\bar{X}_0$, $\bar{X}_1$, $\bar{c}$, $\bar{am}$. Table 2 show, values of density effect correction for (C_2H_4O, C_3H_3N and C_3H_6) as well as the parameter (X).

CONCLUSION

The present calculations refers to that the radiative stopping power (S_{rad}) dominate in range of energy (1-1000) MeV. The density effect correction has

greater effect on the equation Beth-Bloch for calculated collisional stopping power. The stopping time increase with the energy electrons according to multi boundary equations.

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