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ARTICLE

Stopping Power and Range Calculations of Electrons Interaction With C_2H_4 , C_6H_6 and CH_3CHO

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Abstract

The Bethe equation was utilized to ascertain the stopping power, range, and stopping duration of electrons in compounds (C_2H_4 , C_6H_6 , and CH_3CHO) with energies ranging from 0.01 to 1000 MeV. The software MATLAB was utilized in the computation of the results. An equation that exhibited compatibility was identified. A correlation coefficient of 0.999 was calculated, suggesting a strong accord between the obtained results and the outcomes of the E-STAR and SRIM2013 programs. The aim of this manuscript is to present up-to-date mass SPE data, focusing specifically on the characteristics of electron beam therapy (EBT), a technique that directs electrons to the site of a malignant tumor.

Keywords: Stopping power, Range, SRIM-2013 program, Electrons

1. Introduction

C_2H_4 Plant tissue culture is predominately reliant on hormones for the external regulation of morphogenesis. The regulation of the majority of hormones (auxins, cytokinins, and gibberellins) is generally intentional; however, this is not always the case with ethylene, the sole identified gaseous plant growth regulator. Tissue culture necessitates the use of sealed containers, which can lead to changes in gaseous components of plant metabolism, such as ethylene. Consequently, ethylene may constitute an undesirable (contaminant) or unmanageable component of the system [1].

Benzene C_6H_6 , a carcinogenic chemical with extensive application, is positioned within the top 15 chemicals produced globally in terms of volume. It finds application in various industrial processes, encompassing the production of solvents, rubber, and drugs. Additionally, it is generated during the refinement and utilization of petroleum. To mitigate health risks, OSHA and European regulators have established stringent long-term and short-term exposure limits of 1 ppm and 15 ppm, respectively [2].

Acetaldehyde was initially widely employed as an intermediary in the conversion of acetic acid to acetone during World War I. Alcohol, also known as acetaldehyde, is the aldehyde containing the shortest carbon chain. At its center, a carbon atom forms double bonds with an oxygen atom (the carbonyl group), a single bond with a hydrogen atom, and a single bond with another carbon atom (the methyl group) that connects it to three hydrogen atoms. The chemical formula for this substance is CH_3CHO [3].

In the last century, considerable attention has been devoted to comprehending the capacity of charged particles to decelerate and discharge energy. This knowledge has practical implications in numerous fields, including radiology, ion implantation, particle physics, nuclear physics, and radiation damage [4]. In order to accurately calculate the amount of energy that intermediate-energy neutrons deposit in tissue, it is critical to have a thorough understanding of the halting capabilities and projected ranges of low-energy secondary charged particles [5].

Understanding the interaction between radiation and matter This will facilitate the implementation of

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dose restrictions and enhance protective measures, given that radiation therapy is based on the interactions of different forms of radiation with matter, energy dissipation, and the level of radiation exposure that an individual may encounter during medical procedures, accidents, or natural radioactivity [6].

2. Stopping power of electrons

The stopping power of a specific medium is calculated as the mean unit of energy dissipation that charge particles encounter during the course of their journey through that medium. Power cessation involves two components: radiation and collisions. The halting power is predominantly derived from collisions, which occur due to the interaction between particles and atomic electrons. The concept of mass collision stopping power is frequently utilized in order to reduce dependence on the density of the medium [7,8]. A considerable number of physicists have endeavored to ascertain the amount of energy that is lost in matter, as Bethe and Bloch assert. The rate of energy loss is denoted by $(-dE/dx)$, where dE/dx is the energy loss and is a negative integer [9,10].

The collisional stopping-power formulas for electrons and positrons can be written

$$\left(-\frac{dE}{dx}\right)_{col}^{\pm} = \frac{4\pi k_0^2 e^4 n}{m_e c^2 \beta^2} \left[\ln \frac{mc^2 \tau \sqrt{\tau + 2}}{\sqrt{2} I} + F^{\pm}(\beta) \right] \quad (1)$$

Where $F^-(\beta)$ for electron is

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

Here $\tau = T/mc^2$ is the kinetic energy T of the β^- or β^+ particle expressed in multiples of the electron rest energy mc^2 .

To ascertain the appropriate application order of the halting power equations, it is necessary to identify the specific combination of ions and medium being evaluated. With the initial energy of E_0 assumed for an ion, the following equation calculates its total range. A [11].

$$R(E) = \int_E^0 -\frac{1}{S(E)} dE \quad (3)$$

where dE denotes a minimal and restricted amount of energy dissipation, for instance, -0.01 MeV. A particular stopping-power equation is applicable to the energy range DE_1 to DE_2 . (dE/dx) represents the values of the halting powers that are to be derived from the equation at intervals of dE . Until the ion energy reaches E_1 , the calculation

would continue using an additional stopping-power equation that is valid in the energy range of E_1 - E_2 , and so on.

3. Results and discussion

Using the Bethe formula for molecules, the halting power, range, and stopping time were computed. The calculated values are presented in Figs. 1–3, in addition to Table 1. Considering a proton energy range of 0.01–1000 MeV. The Bethe equation was utilized to analyze three distinct compounds, namely CH_3CHO , C_2H_4 , and C_6H_6 .

When electrons pass through matter, they are computed using the same Stopping Power as particles that are highly charged. Computed utilizing Bethe's theory, the "Collisional Stopping Power" signifies the excitation and ionization-causing interaction between incident electrons and atomic electrons. Furthermore, "Bremsstrahlung" electromagnetic radiation is generated due to the acceleration of electrons in the coulomb field of nuclei. "Radiative Stopping Power" is the abbreviation for the corresponding halting force [12].

The graphical depictions (Figs. 1–3) provide visual representations of the halting power calculations that were executed on molecules. The MATLAB software was employed to perform these computations, and the results obtained were contrasted to those obtained from the E-Star software. In order to highlight the distinctions between the curves, coefficients were employed to amplify them, given that they were initially comparable. An appreciable augmentation in halting power was observed for electron energies between $(10^{-2}$ and 1) MeV. The halting force demonstrates a progressive

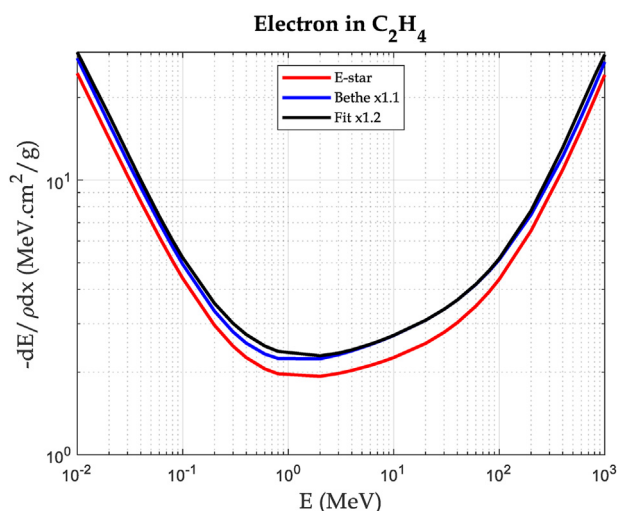


Fig. 1. Stopping power calculations S_{total} for electron in C_2H_4 .

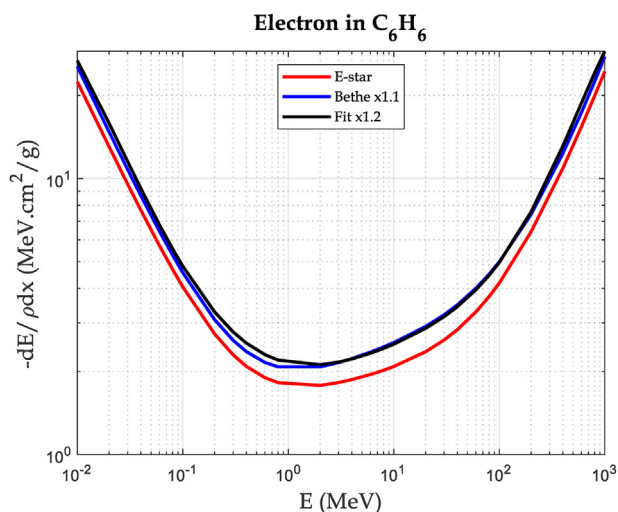


Fig. 2. Stopping power calculations S_{total} for electron in C_6H_6 .

decrease as the energy increases, ultimately attaining a value of 1 MeV, which falls within the precise range of (10^{-2} to 1) MeV. When electrons from the target material obstruct electrons from the projectile, a halting force is produced. A decline in halting power results from the reduction in attenuation in this region, which is caused by an increase in the energy of the discharged electron. Fundamentally, the energy in this region is inversely proportional to the halting power. The braking mechanism

produces the halting force through the transfer of electrons from the medium to the projectile.

It was observed that the energy range of 2 MeV and the electron speed of 29.37 m/s exhibited the greatest halting power, while the energy range of 1000 MeV and the electron speed of 29.99 m/s exhibited the least stopping power. At low energies, the mass stopping capacity of a descending particle increases with its energy. This phenomenon occurs because a positively charged particle undergoes coulomb interactions with the negative electrons and positive nuclei that constitute the atoms of the material as it traverses it. Therefore, due to their low velocity and energy, particles have ample time to engage in inelastic collisions with electrons and nuclei. This can lead to a substantial energy transfer from the moving charged particle to the bound electron through ionization or excitation. This implies that an energetic particle experiences a diminished duration for interaction with atomic electrons and nuclei, leading to a diminished energy dissipation at low energies notwithstanding its high halting power.

The range value of electrons that might undergo loss during their trajectory in compounds (CH_3CHO , C_2H_4 , and C_6H_6 .) was calculated using Equation (3). The data that is obtained is illustrated in Figs. 4–6. Upon conducting an examination of the data, it was discovered that the trajectories demonstrate an

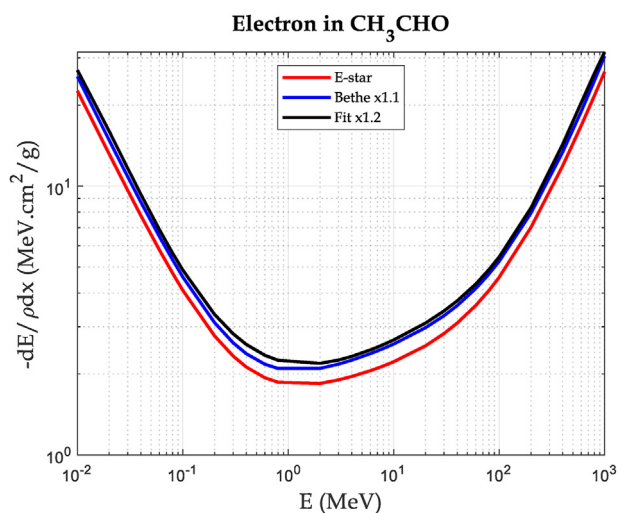


Fig. 3. Stopping power calculations S_{total} for electron in CH_3CHO .

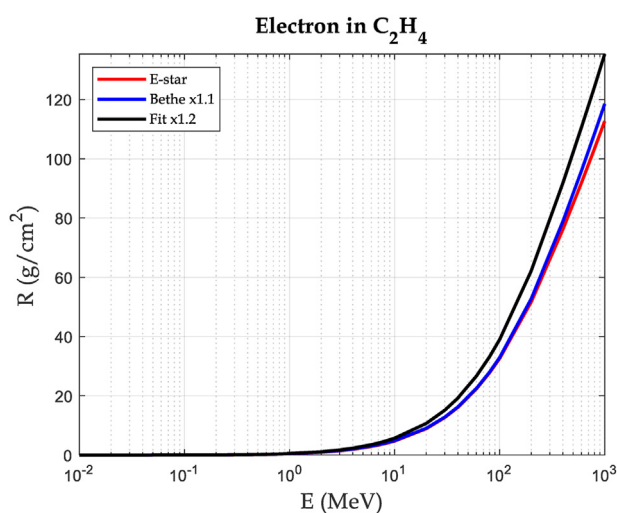


Fig. 4. Rang calculations of electron in C_2H_4 .

Table 1. Correlation and fitting equation for halting power in CH_3CHO , C_2H_4 , and C_6H_6 compounds.

Compound	a	b	c	d	e	f	g	h
C_2H_4	0.287319	-0.079955	0.221828	-0.076082	-0.013037	0.015719	0.000699	-0.000862
C_6H_6	0.253455	-0.081643	0.219420	-0.074031	-0.011284	0.015526	0.000500	-0.000835
CH_3CHO	0.264269	-0.069848	0.226506	-0.074400	-0.012812	0.015454	0.000617	-0.000838

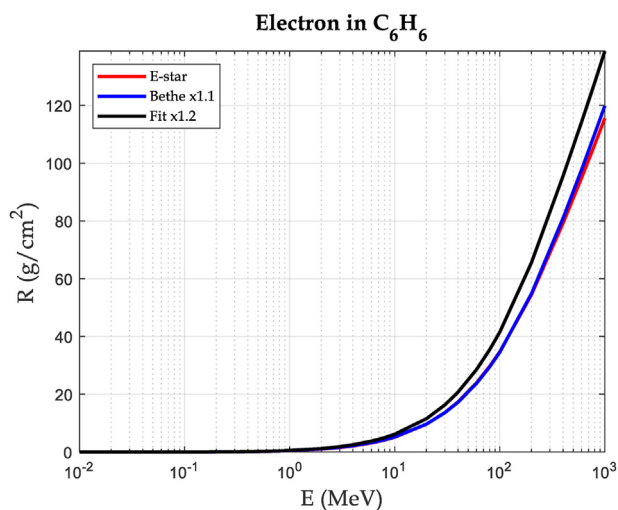


Fig. 5. Rang calculations of electron in C_6H_6 .

inclination towards linearity within the energy range of 0.01%–1.01% MeV. This phenomenon can be explained by the fact that molecules do not deviate substantially upon a single encounter, and interactions occur simultaneously in all directions. After the energy level increases from 12 to 1000 MeV, the spectrum subsequently begins to broaden.

4. The fitting equation

The information was acquired from the SRIM2013 and E-STAR initiatives, and it was analyzed in MATLAB using the Bethe equation. Using the fitting equation in Table 1, an equation representing the halting power in the energy range (0.01–1000) MeV and its constants was derived for the compounds (CH_3CHO , C_2H_4 , and C_6H_6).

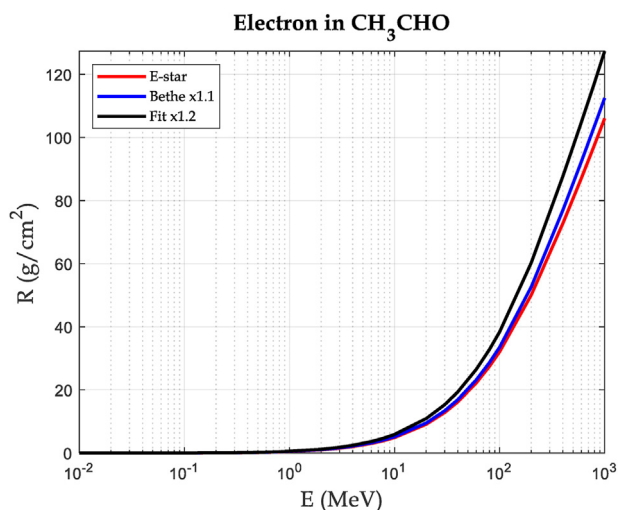


Fig. 6. Rang calculations of electron in CH_3CHO .

5. Conclusion

In contrast, the results of Bethe, MATLAB, and E-Star were evaluated. In light of the initial similarity of the contours, coefficients were utilized to emphasize their differences. A significant augmentation in halting power was observed with the elevation of electron energy from (10-2 to 1) MeV. The halting force exhibits a diminishing trend as the energy increases, reaching a value of precisely 1 MeV within the interval of 10-2 to 1 MeV. The force generated is the result of the impediment that electrons from the target material place on those of the projectile. As electron energy increases, attenuation in this region decreases, leading to a reduction in halting power. Energy and halting power are inversely proportional in this region.

The braking mechanism facilitates the transfer of electrons from the medium to the projectile so as to produce braking force. Trajectories demonstrate an inclination to synchronize within the energy range of 0.01%–1.01% MeV. Distinction in single-contact characteristics among the molecules is minimal, and interactions occur in all directions. The energy level exhibits a further expansion of the spectrum from 12 to 1000 MeV.

References

- [1] Biddington NL. The influence of ethylene in plant tissue culture. *Plant Growth Regul* 1992;II:173–87.
- [2] Geophysical Research Abstracts Vol. 19. EGU2017-11622. A conjugated mess: measurements of benzene (C_6H_6), CH_4 , CO_2 , and H_2O using a cavity ring-down spectrometer Derek Fleck. Santa Clara, CA, USA: John Hoffnagle, and Yonggang He Picarro Inc; 2017.
- [3] ULLMANN'S, an ULLMANN'S encyclopedia of industrial organic chemistry Edition 7, page no. 1987.
- [4] Tufan MC, Gümüs H. Stopping power calculations of compounds by using thomas-fermi-Dirac-weizsäcker density functional. *Acta Phys Pol, A* 2008;114:703–11.
- [5] Al-Affan IAM, Colauti P, Talpo G, Wait DE. Calculated microdose spectra for intermediate energy neutrons (1 to 100 KeV). *Radiat Protect Dosim* 1984;5(3):151–7.
- [6] Tufan MC, Gumus H, Namdar T. Stopping power and CSDA range calculations for incident electrons and positrons in breast and brain tissues. *Springer-Radiat Environ Biophys* 2013:246.
- [7] Kenneths Krane. *Introductory nuclear physics*. Oregon state University; 1987.
- [8] Kenneths Krane. *Introductory nuclear physics*. Oregon stat University; 1987.
- [9] National Research Council. Committee on the biological effects of ionizing radiation, health effects of exposure to low levels of ionizing radiation, BEIR V. Washington, D.C.: National Academy Press; 1990.
- [10] Turner James E. *Atoms, radiation, and radiation protection*, third, completely revised and enlarged edition, 978-3-527-40606-7. 2007.
- [11] Mukherji, Srivastava BK. *Phys. Hev. B* 1974;9:3708.
- [12] Michael FL. *Annunziata ,handbook of radioactivity analysis*. third edition; 2012.