Stopping power calculations for protons

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ABSTRACT In this work we studied the interaction of protons with water. We calculated the stopping power from the theory of Bethe-Bloch equation. We compared the results with the data set of stopping powers from PSTAR and SRIM programs over the energy range from 10 MeV to 250 MeV. The data were plotted and fitted to the empirical formula of Bragg-Kleeman.

1 Introduction

Knowledge of the stopping power is important in many research and applications fields, such as radiation dosimetry, radiotherapy, nuclear physics. etc. Different methods have been reported for measuring, many experimental and theoretical studies about energy loss, stopping power, range have been carried in many different materials The interaction of charged particles with matter has been a subject of study since the early days of atomic physics with Bohr, Rutherford and others . Although, the current theoretical and experimental knowledge is still incomplete When energetic charged particles pass through matter they lost energy due different interactions, these interactions can be ionization, Coulomb interactions, excitation, Bremsstrahlung, , nuclear interactions, etc. These processes result in what we call stopping power, that is defined as the average energy loss per unit path. This deceleration is important in a wide range of fields, such as medical radiation therapy, radiation shielding, fusion. A major advance in understanding stopping powers occurred when Bethe and Bloch derived the fundamental equation for the

2 Theory

For heavy charged particles, such as alpha particle or protons, interact with matter primarily through coulomb forces between their positive charge and the negative charge of the orbital electrons within the absorbed atoms. The following theoretical review will assume the following symbols:

- N_A Avogadro's number
- \bullet r_e Classical electron radius

stopping of very fast particles in a quantized medium, this approach,knew as the Bethe (or Bethe-Bloch) formula, remains the basic method for evaluating the energy loss of particles. We considered two models to calculate the stopping power from the proton energy on diverse materials of medical interest. One of these models is the Bethe formula which is a theoretical formulation, and the Bragg-Kleeman rule, which is an empirical formula based on scaling laws. Both models will be fitted to stopping power values from the PSTAR data-set. We studied the relationship between both formulations for protons on the energy range of 1 Mev - 250 MeV

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- m_e Electron mass
- M Projectile mass
- z Projectile charge (units e)
- Z Atomic number of absorber
- A Atomic mass of absorber
- I Mean excitation energy
- E Particle energy
- v Particle velocity
- v_0 Bohr velocity $\frac{e^2}{h}$
- b impact parameter of particle to a target electron
- N Density of target atoms per unit volume
- β Relative particle velocity $\frac{v}{s}$
- c Speed of light

The next assumptions has to be made in order to The particle is assumed to interact only through electromagnetic forces and the mass of the particle M is much greater than the electron mass m_e . So in the classical Bohr approach considers a heavy charged particle of charge ze, mass M, moving at a velocity, v, passing through a target of charge Ze then we have that the energy transfer onto a target with mass m_t is given by

$$\Delta E = \frac{\Delta p}{2m_t} \tag{1}$$

Then its momentum transfer time integral is

$$\Delta p = \int_{\infty}^{\infty} F_c dt \tag{2}$$

where F_c is the Coulomb force

$$F_c = \frac{1}{4\pi\epsilon_0} z Z e^2 / r^2 \tag{3}$$

And since the longitudinal forces cancel due symmetry $F_l(x) = -F_l(-x)$ only transverse forces F_t

 $F_c \cdots \frac{b}{|r|} = F_c cos\theta$ have a contribution. Now taking $r = b/cos\theta$ we have that the transverse forces on projectile are

$$F_{ct} = \frac{1}{4\pi\epsilon_0} \frac{zZe^2}{r^2} cos\theta = \frac{1}{4\pi\epsilon_0} \frac{zZe^2}{b^2} cos^3\theta \qquad (4)$$

then the momentum transfer onto target

$$\Delta p(b) = \int_{-\infty}^{\infty} F_{ct} = \int_{-\infty}^{\infty} F_{ct} \frac{dx}{v} = \frac{1}{4\pi\epsilon_0} \frac{zZe^2}{b^2} \int_{-\infty}^{\infty} \cos^3\theta \frac{bd\theta/\cos^2\theta}{v}$$

$$(5)$$

$$1 \quad zZe^2 \quad f^{\pi/2} \qquad (2)$$

$$=\frac{1}{4\pi\epsilon_0}\frac{zZe^2}{bv}\int_{-\pi/2}^{\pi/2}\cos\theta d\theta = \frac{1}{4\pi\epsilon_0}\frac{2zZe^2}{bv} \qquad (6)$$

Thus the energy transfer onto target with mass m is given by

$$\Delta E(b) = \frac{\Delta p^2}{2m} = \frac{2z^2 e^4}{m_e c^2 \beta^2 b^2}$$
 (7)

in this case taking the shell electron as Z=1 and $m_t=m_e$. Now we sum over all shell electrons and integrate over all collision parameters b considering the energy loss due to collisions with electrons in tube of length dx and thickness db at radius b. Also we define the number of electrons as $2\pi b db dx N_e$ and the electron density as $N_A Z/A\rho$ then

$$-dE(b) = \Delta E(b)N_e dV = \frac{4\pi z^2 e^4}{m_e c^2 \beta^2} N_e \frac{db}{b} dx \qquad (8)$$

integrating over collision parameter from b_min to b_{max} we have

$$\frac{-dE}{dx}(b) = \frac{4\pi z^2 e^4}{m_e c^2 \beta^2} \rho N_A \frac{Z}{A} \frac{1}{b}$$
 (9)

then

$$\frac{-dE}{dx} = \frac{4\pi z^2 e^4}{m_e c^2 \beta^2} \rho N_A \frac{Z}{A} ln \frac{b_{max}}{b_{min}}$$
(10)

where $b_{min} = \frac{ze^2}{\gamma m_e c^2 \beta^2}$ and $b_{max} = \frac{ze^2}{c\beta} \sqrt{\frac{2}{m_e I}}$ since the maximal energy transfer for a central collision is given by

$$\Delta E(b) = 2\gamma^2 m_e \beta^2 c^2 = \frac{2z^2 e^4}{m_e c^2 \beta^2 b^2}$$
 (11)

finally we have that the classical formula for energy loss due to ionisation can be expressed as

$$\frac{-dE}{dx} = \frac{Kz^2\rho}{\beta^2} \frac{Z}{A} \frac{1}{2} ln \frac{2c^2\gamma^2\beta^2 m_e}{I}$$
 (12)

where $K = \frac{4\pi e^2}{c^2 m_e} N_A$ After the works realized by Bloch and Bethe we can express the full quantum mechanical derivation that describes the mean energy loss or stopping power as

$$-\frac{dE}{dx} = Kz^{2} \frac{Z}{A} \frac{1}{\beta^{2}} \left[\frac{1}{2} ln \frac{2m_{e}c^{2}\beta^{2}\gamma^{2}T_{max}}{I^{2}} - \beta^{2} \right]$$
(13)

where $K = 4\pi N_A r_e^2 m_e c^2$ with N_A the Avogadro's number, r_e the classical electron radius, $m_e c^2$ the electron mass in MeV, z is the particle charge in terms of e, /rho, Z the atomic number of the medium, A the atomic mass of the medium, I the mean excitation energy and

$$\beta = \frac{v}{c} = \frac{p}{E} = \frac{\sqrt{E^2 - m^2 c^4}}{E} \tag{14}$$

is the relativistic velocity where E is the rest energy of the incident particle and and p the particle's momentum, and

$$\gamma = \frac{1}{\sqrt{1 - \beta^2}} \tag{15}$$

the Lorentz factor, and finally we have that

$$T_{max} = \frac{2m_e c^2 \beta^2 \gamma^2}{1 + \frac{2\gamma m_e}{M} \left(\frac{m_e}{M}\right)} \tag{16}$$

We solved it through numerical integration for protons in a range of energies from 1-250 MeV. Now we define the range of a particle as the distance between the initial and final point (after being absorbed by the medium) of the incident particles or as the relation between the initial energy and the depth of the medium, given according to the continuous-slowing-down approximation (CSDA) by:

$$R = \int_0^{E_0} \frac{dx}{dE} dE \tag{17}$$

Another formulation to calculate the stopping power

is given by the Bragg-Kleeman rule which define the proton range by:

$$R = \alpha E_0^p \tag{18}$$

where E_0 is the initial energy of the proton, α is a material dependent constant and p is a constant that depends on the proton energy also known as Geiger's rule. From this expression we can obtain the stopping power. The protons deposits energy along its path between x=0 and x=R in the medium. The remaining energy E(x) at an arbitrary depth x must be sufficient to travel the distance R-x thus

$$E(x) = \left(\frac{R-x}{\alpha}\right)^{\frac{1}{p}} \tag{19}$$

then differentiating the energy with respect x we have:

$$-\frac{dE}{dx} = \frac{E^{1-p}}{\alpha p} \tag{20}$$

We will use both models to fit the data obtained from PSTAR and SRIM .

3 Methods

To obtain a relationship between both models we decided to use the PSTAR data-set constructed by the United states National Institute of Standards and Technology (NIST). It consist of mass stopping powers for a large range of proton energies from a variety of elements and compounds most of them commonly present in biological tissues. The total stopping power is calculated from the sum of the electronic stopping power (due Coulomb interactions) and nuclear stopping power (due to elastic scattering with atomic nuclei) but because the interactions taking into account on this project we noticed that only the electronic stopping power has a significant contribution on the total stopping power. The stopping powers from the data-set for energies from 1 to 250 MeV will be fitted to both stopping power formula as a function of energy. All fits are made using a Python script that uses a least square method, the error of both fits will be compared. The free parameters used for fitting are α , and . We also computed the stopping power, range and exit energy from Bethe formula with a numerical iterative method using a python script and compared the results with both fits.

4 Results

The electronic stopping power for heavy charged particles has been calculated numerically. Protons lose their energy due to the collisions with the atomic electrons of the absorbing material. The stopping power was also obtained by using two simulation techniques. From figure 1 it, it is observed that there is a significant reduction in the energy range of 1 MeV to 50 MeV Now the Bethe-Bloch equation as stated above

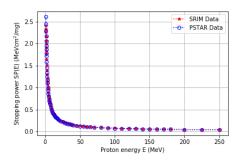


Figure 1: Electronic stopping power for a proton in water:results obtained by PSTAR by NIST and SRIM simulations methods

has units of [MeV/cm] and is a function of energy. In this project it was obtained by numerically integrating over a energy range from 1 MeV to 250 MeV, which from it is clear that the energy lost by a charged particle is inversely proportional to the square of its velocity. This can be seen on the term $\frac{1}{\beta^2}$ on the equation. Then we proceed to fit the data from PSTAR to the Bragg-Kleeman rule with α and p as fitting parameters using a least square method. On the table 1 we present the values of the fit, they

Par.	Estimate	Std. dev	Mean R
р	1.76	0.003	0.99
α	0.46	0.002	0.99

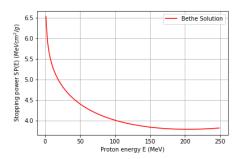


Figure 2: Stopping power from a proton in water obtained by Bethe-equation

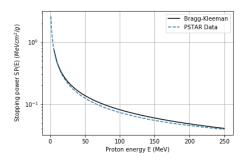


Figure 3: Bragg-Kleeman fitted to PSTAR data

agree with the ones found in the literature for the range of 1-250 MeV We followed a similar procedure to fit the data to the Bethe model and compared with the Bragg-Kleeman fit.

The parameters that we obtained were. We found

Par.	Estimate	Std. dev	Mean R		
I	7.51e-05	1.10e-11	0.99		
p	1.11	0.001	0.98		
α	0.75	0.045	0.98		

that they have a good agreement with what we expected.

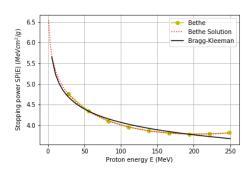


Figure 4: Data fitted to both models

5 Conclusion

After considering both the Bragg-Kleeman rule and the Bethe-Bloch formula we concluded that the Bethe formula is the most appropriate and has only a free fitting parameter which makes it easy to work with, on the other hand the Bragg-Kleeman rule gives a good approximation for the range of energies on we were interested and it is easier to manipulate numerically. Comparing to the physical basis and the stopping power values of the PSTAR and the SRIM dataset showed that there is not much difference between the two, so any of both can be used .

References

- [1] J. Kiusalaas, Numerical methods in engineering with Python 3 (Cambridge university press, 20 13).
- [2] Hooshang Nikjoo, Shuzo Uehara, Interaction of Radiation with Matter, (CRC press, 20 12).
- [3] J. F. Ziegler. "The stopping of energetic light ions in elemental matter. Journal of applied physics", (1999).
- [4] Ziegler, J.F., M.D. Ziegler, and J.P. Biersack, SRIM: the stopping and range of ions in matter. 2008: Cadence Design Systems.

- [5] Physics.nist.gov. (2020). https://physics.nist.gov/PhysRefData/Star/Text/PSTAR.html
- [6] Borthfeld, T., Schlegel W. "An Analytical approximation of deepth-dose distributions for therapeutic proton beams". Phys. Med. Bio 41 1331, (1996)
- [7] Grimes D.R, Warren D. R, Partridge M. "An approximate analytical solution of the Bethe equation for charged particles in the radio therapeutic energy range". Nature Scientific reports, (2017)
- [8] Glenn F. Knoll, Radiation Detection and Measurement, (John Wiley Sons, Inc., Third edition 20 10).

https://docs.scipy.org/doc/ scipy/reference/generated/scipy.optimize.curve_tit.html