Method for range calculation based on empirical models of proton in liquid water: Validation study using Monte-Carlo method and ICRU data.

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Abstract— The biological damages are mainly produced by direct ionization and excitation of bio-molecular DNA electrons or by indirect chemical reaction of water radiolysis products with DNA. In this work, we restricted our study on the interaction of energetic ion proton beams with liquid water; since the water represents over 80% of the most-soft tissues. The proton collisions with water molecules are estimated from the ionization, excitation, and charge-changing processes. We studied the Bragg-Kleeman rule $R = N \times E^{\beta}$, between the range ***(R)*** and the incident kinetic energy ***(E)***, in the range of 1 − 300 MeV. We also approximated the range-energy relationship from a fourth degree polynomial. The Bragg peak profile and position (range) were determined from an analytical approach. The obtained results were compared with the experimental data from ICRU and the calculated ones from Monte-Carlo method using GEANT4-DNA, SRIM and DOSIMEX toolkits. The results are in well agreement to be used a basis for a forwarded estimation of the Bragg peak in the biological material H_2O + DNA.

Index Terms— Biological damage, Water, Charge changing, Excitation, Ionization, Bragg peak, Bragg-Kleeman, Range.

1 INTRODUCTION

The interaction of charged particles with bio-molecular tissues is one of the most investigated technique of modern radiation therapy used in cancer treatments. The advantage of such particle therapy technique is demonstrating in the specific deposited energy on the targeted place in the body and hence the tumor is completely destroyed with minor secondary effects on the surrounding cells. The high-energy proton therapy is the most intensively used technique, in the last decade, and hence-after an understanding literature works have started to study the physics and the biological consequences of the interaction of proton beam with matter [21]. To quantify the effects of ionizing radiation it is important to know how its energy is distributed linearly. Since the liquid water represents 70-80% of all biological matter, it is, therefore, important to study the physical processes and the induced radiolysis of intracellular water molecules.

This work focuses the physical processes of the interaction of proton beam with liquid water molecules. A review of differential cross sections of excitation, ionization, charge-changing, elastic and inelastic scattering processes mainly dominates the energy loss per unit length of traveling protons through the matter.

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For an impinging high-energy proton, the whole energy is completely deposited in a sharp position at the end of trajectory, which is so-called the Bragg-peak. Therefore, the range and the shape of Bragg-peak are the most important parameters to characterize in term of stopping power, which is the energy loss per unit path length in material. The IAEA report [5] presents, by far, the most comprehensive database of doubly differential cross sections that could be emphasized with such numerical model. Hebert et al. [3] and Inokuti [6] have emphasized this database to be useful for radiological applications. Several theoretical and semi-empirical works [13] are investigated to compute the stopping power Bragg-peak position of proton beams with water and DNA. The Molinas approach [4], modelized the stopping power as a function of target depth in liquid water for proton beams with incident energy ranging from 0.5 to 10 MeV/u. In the same way, Rudd et al [17], Miller and Green [13], Zaider et al [26] and Emfietzoglou et al [14] have developed semi-empirical models for proton ionization and interaction cross sections for liquid and vapor water, taking in account the contribution of sub-shell ionization of water molecule.

In this work, we use the different semi-empirical models to numerically compute the differential cross sections of the interaction of proton beam with liquid water. In our analytical approach, the incident beam is treated event by event and the target medium is discretisized, incremented, and divided into layers. The thickness of each layer is selected randomly from a distribution weighted by the values of the total interaction cross section. We compute the

electronic and nuclear stopping powers for a large variety of proton beams ranging the energy of 1- 300 MeV. We compare our computed results with the published data from ICRU [5]. We study the Bragg-Kleeman rule, $R = N \times E^{\beta}$, between the range (R) and the incident kinetic energy (E). We emphasize our analytical results with the analytic ones obtained by Ulmer [25] and the Monte Carlo calculations using GEANT4-DNA, SRIM and DOSIMEX toolkits [24].

Finally, since the liquid water is considered an excellent tissue substitute owing to its similar density and other properties, the aim is to emphasize the Bragg-Kleeman rule between our analytical approach and Monte-Carlo method for further study and applications of proton beam with biological material of H_2O + DNA.

2 Proton Interactions With Liquid Water

2.1 Proton impact cross sections

The transport of charged particle through the matter may follow many collision processes leading to the energy loss of the incident particle. In the case of interaction of proton beam with liquid water, the main physical processes could be represented from the reaction mechanisms of:

Ionization by proton: $p + H_2O \rightarrow p + H_2O^{+} + e^{-}$
Excitation by proton: $p + H_2O \rightarrow p + H_2O^{*}$
Electron capture: $p + H_2O \rightarrow H + H_2O^{+}$
Ionization by hydrogen: $H + H_2O \rightarrow H + H_2O^{+} + e^{-}$
Excitation by hydrogen: $H + H_2O \rightarrow H + H_2O^{-}$
Stripping of hydrogen: $H + H_2O \rightarrow p + H_2O + e^{-}$

The cross section corresponding of each so-called interaction is called a partial cross section, and the sum of all differential cross sections is the total cross section. Several empirical approaches have been developed to treat each type of differential cross section [11, 12, 14, 23].

2.1.1 Ionization cross section

The induced ionization by proton with initial energy E_0 is the dominant process contributing to the energy loss and resulting in the production of the secondary electrons, with ejected energy of W. We use the semi-empirical expression developed by Rudd et al [17, 19] to calculate the singly differential cross section at each impact with the electrons of liquid water. For the consideration of five molecular orbitals of a water molecule, the differential cross section is expressed:

$$\frac{d\sigma_{ion}(W,E_0)}{dW} = \sum_i^5 S_i \frac{F_1(\nu_i) + F_2(\nu_i)\omega_i}{(1+\omega_i)^3\left(1+\exp\dfrac{\alpha(\omega_i-\omega_i^{\max})}{\nu_i}\right)} \quad (1)$$

And

$$S_i = z^2 \frac{4\pi a_0^2 N_i}{I_i}\left(\frac{R}{I_i}\right)^2 \quad (2)$$

Where a_0 = 0.0529 nm is the Bohr radius, R = 13.6 eV is the Rydberg constant energy, I_i is the binding energy of the electron sub-shell i, N_i is the shell occupancy, $\omega_i = \frac{W}{I_i}$ is the scaled secondary electron energy, $\nu_i = \sqrt{\frac{E_{ion}}{I_i}}$ is the dimensionless normalized velocity, E_{ion} is the energy of an electron of mass m which would have the same velocity as a proton of mass M of the same energy $E_{ion} = E_0(m/M)$, $\omega_{ion}^{\max}$ is the scaled cutoff energy $\omega_{ion}^{\max} = 4\nu_i^2 - 2\nu_i - (R/4I_i)$, $\alpha = 0.64$ is a numerical parameter related to the relative size of the target molecule.

The functions $F_1(\nu)$ and $F_2(\nu)$ are expressed as fellow:

$$F_1(\nu_i) = L_1(\nu_i) + H_1(\nu_i) \Rightarrow \begin{cases} L_1(\nu_i) = \dfrac{C_1 \nu_i^{D_1}}{1 + E_1 \nu^{(D_1+4)}} \\ H_1(\nu_i) = \dfrac{A_1 \ln(1+\nu_i^2)}{\nu_i^2 + \dfrac{B_1}{\nu_i^2}} \end{cases} \quad (3)$$

$$F_2(\nu_i) = \frac{L_2(\nu_i)H_2(\nu_i)}{L_2(\nu_i)+H_2(\nu_i)} \Rightarrow \begin{cases} L_2(\nu_i) = C_2 \nu_i^{D_2} \\ H_2(\nu_i) = \dfrac{A_2}{\nu_i^2} + \dfrac{B_2}{\nu_i^4} \end{cases} \quad (4)$$

And, the parameters sets of A_j, B_j, C_j, D_j (j = 1, 2) for liquid water were found in the Refs [11, 12].

The differential cross section is adjusted by Rudd et al [20] by adding a partitioning factor G_j which takes into account the contribution of sub-shells:

$$\frac{d\sigma_{ion}^i}{dW} = \sum_i^5 G_i \frac{d\sigma_i}{dW_i} \quad (5)$$

The total ionization cross section is numerically computed from the integral:

$$\sigma_{ion} = \int_0^{W_{\max}+I_i} \left(\frac{d\sigma_{ion}^i}{dW}\right) dW \quad (6)$$

Where $W_{max} = E_0 - I_i$ is the maximum kinetic energy of the ejected electron.

2.1.2 Excitation by protons

The incident protons lose mainly their energy by Coulomb interactions with the outer shell electrons of water molecules causing the excitation or ionization processes. For the excitation processes, we use for each sub-shell electron l the semi-empirical expression from the Refs [11,13]:

$$\sigma_{exc,l}(E_0) = \frac{\sigma_0 (Za)^{\Omega} (E_0 - E_l)^{\nu}}{J^{\Omega+\nu} + E_0^{\Omega+\nu}} \quad (7)$$

Where $\sigma_0 = 10^{-20} m^2$, Z = 10 is the number of electrons, E_l is the excitation energy. The parameter values of a, J, Ω and ν,

set for liquid water can be found for all the five excited states in the Ref [11].

2.1.3 Electron capture

At the end of range, the incident proton causes maximum interactions with outer electrons of water molecules. For residual energy E_0 less than 100 keV, the incident protons can capture or exchange electrons with hydrogen atoms of water molecules. We use the electron capture cross section σ_{10} proposed by Rudd et al [15], represented by the harmonic mean of high-energy part σ_{high} and low-energy part σ_{low}:

$$\sigma_{10}(E_0) = \sigma_+(E_0) - \sigma_-(E_0) \quad (8)$$

Where $\sigma+$ and $\sigma-$ are respectively the production cross section of positive and negative charge. They are given by:

$$\sigma_{\pm}(E_0) = \left(\frac{1}{\sigma^{\pm}_{low}} + \frac{1}{\sigma^{\pm}_{high}} \right)^{-1} \quad (9)$$

$$\sigma^{\pm}_{low}(E_0) = 4\pi a_0^2 \left(C^{\pm} x^{D^{\pm}} + F^{\pm} \right) \quad (10)$$

$$\sigma^{\pm}_{high}(E_0) = 4\pi a_0^2 \left(\frac{A^{\pm} \ln(1+x) + B^{\pm}}{x} \right) \quad (11)$$

Where $x = T/R$, R is Rydberg energy, $T = E_{ion}/M_p$, T is the kinetic energy of an electron travelling at the same speed as the proton and M_p is the mass of proton. a_0 is the Bohr radius. $A^{\pm}$, $B^{\pm}$, $C^{\pm}$, $D^{\pm}$ and $F^{\pm}$ are fitted parameters as given by Rudd [17, 18].

2.1.4 Ionization and excitation by neutral hydrogen

At low-energy below the proton's stopping power the electron capture becomes very probable and leading to the creation of hydrogen with an important initial energy. The ions and radicals hence produced by both electron capture can induce biological damage in the bio-molecules such as DNA effectively [10, 15, 21]. However, in spite of their importance, the cross section measurements for molecular water ionization by neutral hydrogen impact remain extremely rare. Many semi-empirical models were then proposed to overcome the lack of theoretical support. We use the model developed by Dingfelder et al. [11] to numerically calculate the differential ionization cross section for neutral hydrogen impact:

$$\left(\frac{d\sigma_{ion}}{dW} \right)_{Hydrogen} = g(E) \left(\frac{d\sigma_{ion}}{dW} \right)_{Proton} \quad (12)$$

Where $g(E)$ is adjusted by Dingfelder and co-workers [9] to fit the values for liquid water provided by ICRU [5]. And,

$$g(E) = 0.8 \left[1 + \exp\left(\frac{\log(E) - 4.2}{0.5} \right) \right]^{-1} + 0.9 \quad (13)$$

Where $g(E)$ is weighting constant $(0.9 \le g(E) \le 1.7)$. However, the excitation of water molecule by neutral hydrogen impact is neglected in many studies. In this work, we consider that the hydrogen like-beam may cause excitations as well as the protons. We use the cross section proposed by Miller and Green [11] which can take the expression of equation 13 except the parameter a assumed to be three-quarters of the proton value corresponding to the effective charge of proton with the screen effect of the bounded electron in hydrogen atom [9].

2.1.5 Stripping by neutral hydrogen

The neutral hydrogen can undergo stripping or electron-loss. We use the stripping cross section evaluated from the analytical functions developed by Miller and Green [13] and fitted to the experimental data of Toburen et al.[23] and Dagnac et al. [1]. The loss of electron is estimated from the semi-empirical formula:

$$\sigma_{01}(E) = \frac{\sigma_0 (Za)^{\Omega} (E - I)^{\nu}}{J^{(\Omega+\nu)} + E^{(\Omega+\nu)}} \quad (14)$$

$Z = 10$ is the number of electrons in the target molecule, E is the proton energy, $I = 12.6$ eV is the ionization threshold, v = 0.943 and Ω = 0.652 are dimensionless parameters, a = 79.3keV and J = 27.7keV are parameters with the dimension of energy.

2.1.6 Total cross section

The differential cross sections of different physical processes cited above are plotted in Fig. 1 for an incident proton beam of energy ranging from 10 eV to 100 MeV. As we can observe from the figure, the electron capture process is dominant at low energy till intermediate one of 100 keV. For high energy, the dominant processes are the ionization and stripping.

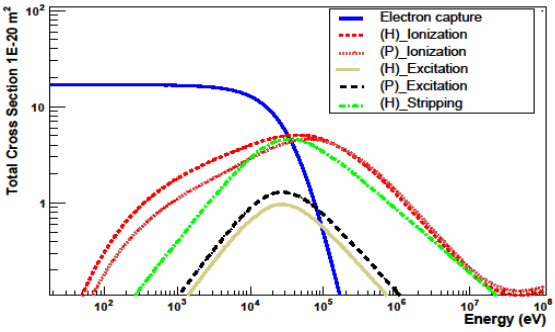

Fig 1: Total cross sections of the considered inelastic processes of protons in liquid water.

2.2 Calculation of stopping cross section for protons

The energy loss of proton beam is basically related with the elementary component of the traversed medium. It depends on the charge and velocity of the incident charged particles and the atomic and electron density of the target material. It is therefore convenient to express the energy loss rate of incident ions in term of stopping power, which is defined as the quotient of:

$$S(E_p) = \frac{dE}{dx} = N\sigma_{sct}(E_p) \quad (15)$$

Where dE is the mean energy loss, dx is the traversed distance in target material, E_p is the incident proton energy, N is the number of water molecules per unit of volume (= 3.342×10^{28} m^{-3}), and σ_{sct} is the total stopping cross section [4, 9]:

$$\sigma_{sct} = \varphi_0\sigma_{sct,0} + \varphi_1\sigma_{sct,1} + \sigma_{sct,CC} \quad (16)$$

Where $\sigma_{sct,CC}$ is the charge changing stopping cross section, φ_0 and φ_1 are respectively, the probability of finding the incident particle like-hydrogen or like-proton particles, they are expressed as [11]:

$$\varphi_0 = \frac{\sigma_{10}}{\sigma_{10}+\sigma_{01}} \;;\; \varphi_1 = \frac{\sigma_{01}}{\sigma_{10}+\sigma_{01}} \quad (17)$$

σ_{01} and σ_{10} represent respectively the cross section of the electron capture and the electron loss processes, σ_{01} is calculated by using the Miller and Green semi-empirical formula [13] and σ_{10} is the electron capture cross section as given by the semi-empirical formula from Rudd et al., [18].

In Fig. 2, we show the gradual depletion of protons from entrance to near the end of range in terms of probability of finding the incident particle in the neutral state, φ_0, and the charge state, φ_1. At low energy the neutral state like hydrogen becomes more important.

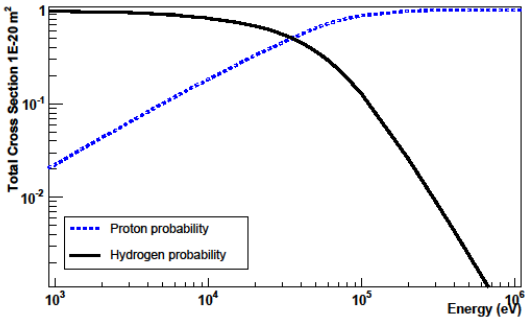

Fig 2: The probability to find the projectile as neutral hydrogen.

2.2.1 Electronic stopping cross section

The total stopping cross section $\sigma_{st,i}$ is defined as the sum of the ionization and the excitation stopping cross section of the incident particle as a function of the charge state i ($i = 1$ for the proton and $i = 0$ for the hydrogen).

$$\sigma^i_{sct} = \sigma^i_{sc,ion} + \sigma^i_{sc,\text{exe}} \quad (18)$$

The ionization stopping cross section for the incident particle for a charge state i, is given by:

$$\sigma^i_{sc,ion} = \sum_j G_j \int_0^{W_{\max}+I_j} (W + I_j)\left(\frac{d\sigma^j_{ion}}{dW}\right)_i dW \quad (19)$$

Where G_j is the partitioning factor to adjust the contribution of different sub-shells j; W is the energy of the secondary electrons, and I_j is the binding energy of the electron in the sub hell j of the water molecule.

The charge changing process is given by the following formula [13]:

$$\sigma_{st,CC} = \frac{\sigma_{10}\sigma_{01}}{\sigma_{10}+\sigma_{01}}(I_0 + T) \quad (20)$$

I_0 is the ionization energy of water molecule where T is given as: $T = \frac{m_e}{M_p}E_p$. The ionization and the excitation stopping cross sections are given by:

$$\sigma^P_{st,exe} = \sigma^P_{exe}T_{11} \quad (21)$$

$$\sigma^H_{st,exe} = \sigma^H_{exe}T_{00} \quad (22)$$

T_{11} and T_{00} are the amount of the energy loss during the excitation and the ionization process.

We show in Fig. 3 the stopping power calculated for all the considered inelastic processes as function of incident energy below 100 MeV/n. We note the dominance of ionization process for proton at high energy till 1 keV. For low energy less than 300 keV, the ionization by neutral hydrogen and the charge-changing processes become more dominant than the excitation process. The total stopping cross section is therefore represented in good agreement with the ICRU recommended values [5].

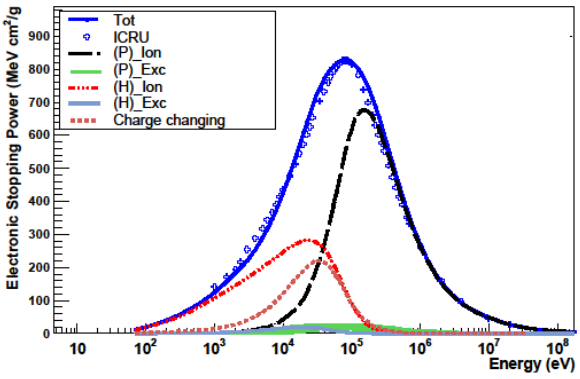

Fig 3: Stopping cross sections for different processes and total stopping cross section of energetic protons passing through a volume of water.

2.2.2 Nuclear stopping power calculations

The nuclear stopping power in liquid water for proton with incident energy of E_p, was semi-empirically developed by Ziegler et al [27, 28] as given by:

$$S_n(E_P) = \frac{8,462.10^{-17}.Z_1.Z_2.M_1}{(M_1+M_2).(Z_1^{0,23}+Z_2^{0,23})}.S_n(\varepsilon) \quad (23)$$

Where M_1 and M_2 are the projectile and target masses (amu), respectively, Z_1 and Z_2 are the projectile and target atomic numbers, respectively. ε is the reduced proton energy expressed as follow:

$$\varepsilon = \frac{32,53.M_2}{Z_1.Z_2.(M_1+M_2).\left(Z_1^{0,23}+Z_2^{0,23}\right)}.E_P \qquad (24)$$

The analytical approximation for $S_n(\varepsilon)$ is given by:

$$S_n(\varepsilon) = \begin{cases} \dfrac{\ln(1+1,1383.\varepsilon)}{2.\left(\varepsilon+0,01321.\varepsilon^{0,21226}+0,19593.\varepsilon^{0,5}\right)} & for\ \varepsilon \le 30 \\ \dfrac{\ln(\varepsilon)}{2.\varepsilon} & for\ \varepsilon \ge 30 \end{cases} \qquad (25)$$

In the present work, we consider the contribution of the nuclear stopping power. As we can see from the Fig. 4, the elastic and inelastic nuclear processes could contribute even less on the stopping power of incident charge particles. The nuclear stopping power is significant at the end of incident trajectory, with maximum value rarely exceeding 20% of the electronic power, and it is negligible for incident energy above 200 keV/n [7, 8]. Therefore, the total stopping power is the sum of both electronic and nuclear stopping power, even the contribution of the last is weak. The shape and position of Bragg peak is hence-after demonstrated by the behavior of total stopping cross section. The results of our work are in good agreement with ICRU recommended data [5].

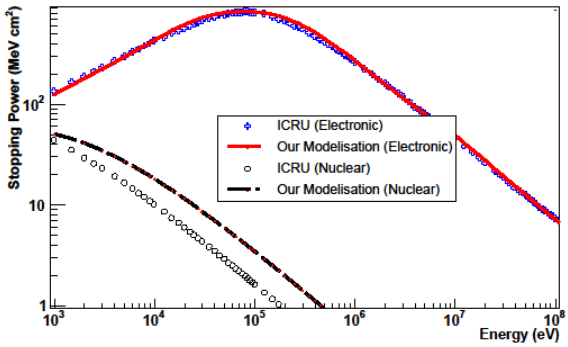

Fig 4: Stopping cross sections for Nuclear and Electronic processes of energetic protons passing through a volume of water

3 Depths of Bragg Peak Calculations

The energy loss per unit length defined as the stopping power evolutes gradually with greater depth and lower speed, and suddenly rises in a short position (Bragg peak) where the proton is completely stopped. The slowing down of proton to inferior limit of 14 eV can be written when we only consider the electronic interaction as:

$$E_p^i(x) = E_p^0 - \sum_{j=1}^{i-1} S_E\left(E_p^j\right)x_j \qquad (26)$$

And the nuclear and electronic interactions as:

$$E_p^i(x) = E_p^0 - \sum_{j=1}^{i-1} S_{E+N}\left(E_p^j\right)x_j \qquad (27)$$

Where S_{E+N} is the sum of electronic and nuclear stopping power for proton with incident energy of E_p^0, E_p^j is the residual energy of proton traveled x_j, defined as the flight distance between two successive collisions, which is given by Date et al. [2]:

$$x_j = \frac{-\ln\xi}{\sigma_{tot}^j N} \quad and \quad R_{range} = \int_0^L dx = \sum_{j=1}^{i-1} x_j \qquad (28)$$

Where σ_{tot}^j, is the total collision cross section for each gradient of energy E_p^j, $N=3.34\times10^{28}$ is the density of water molecules and ξ is a random number ($0<\xi<1$). The total collision cross section consists of ionization, excitation by proton and neutral hydrogen, and charge-changing processes (electron capture and stripping). R_{range} is the total depth traveled by proton in water.

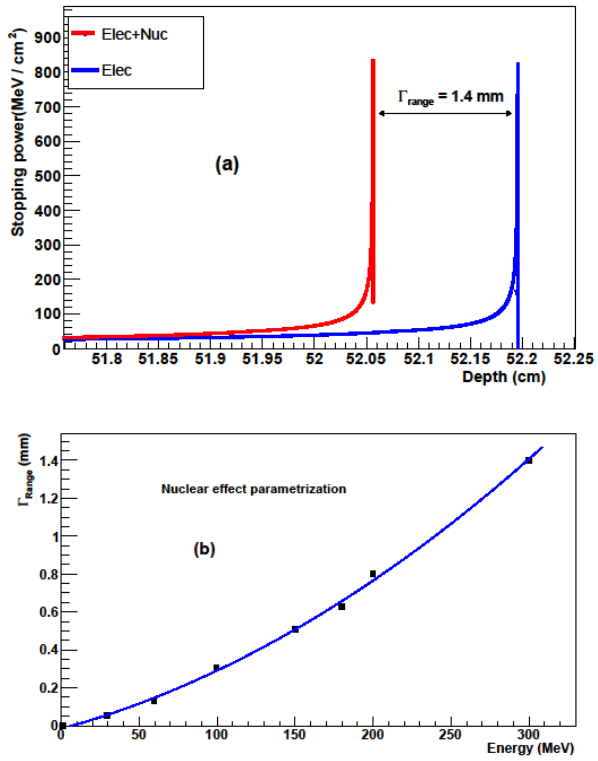

Fig 5: **(a)** Depth of Bragg peak with only electronic and both electronic and nuclear interactions for protons with incident energy of 300 MeV. **(b)** The contribution of nuclear stopping power on the depth of Bragg peak.

We show in Fig. 5**a**, the Bragg curves with and without consideration of nuclear collisions for protons with incident energy of 300 MeV in liquid water. We estimate the contribution of nuclear interactions in terms of Γ_R defined as the difference between ranges, $\Gamma_R = R_{Elec} - R_{Elec+Nuc}$, of equations 25, 26 of 27. We studied the correlation of Γ_R as a function of incident energy from 0 to 300 MeV. We show in Fig. 5**b** the non-linearity of nuclear stopping power

contribution. We parameterize the correlation of Γ_R as a function of:

$$\Gamma_R = \sum_{a=0}^{2} \alpha_a E_p^a \qquad (29)$$

Where α_0, α_1, α_2 are a set of parameters with fitted values of $\alpha_0 = -6.16764\text{x}10^{-03}$, $\alpha_1 = 1.93421\text{x}10^{-03}$ and $\alpha_2 = 9.10485\text{x}10^{-06}$.

However, in the previous work of Ulmer [25] the CSDA (Continuous Slowing Down Approximation) range is calculated by integrating the inverse of the linear stopping power of the proton from zero to the initial energy. It results from a generalized (non relativistic) Langevin equation and a modification of the phenomenological friction term. In this work, we calculate the range from the equation 27 and the stopping power using the equation 26. In Fig. 6, we show together the profiles of range and total stopping power for proton with incident energy of 300 MeV in liquid water.

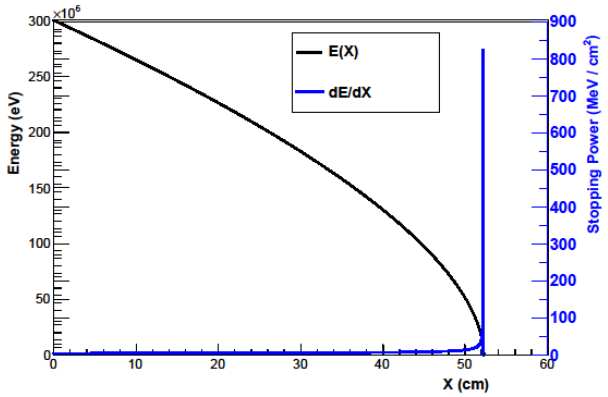

Fig 6: The E(x) and dE(x)/dx as a function of x = Range (cm).

Using this result we can estimate the proton depth in another medium that is of importance when we want to add the DNA to our analysis. This estimate can be parameterized by this equation:

$$X_{medium} = X_{water} \left(\frac{Z_\rho}{A_N}\right)_{water} \left(\frac{A_N}{Z_\rho}\right) \qquad (30)$$

For water we used $Z = 10$, the nuclear charge, $A_N = 18$, mass number, $\rho = 1g \times cm^{-3}$, density (Bragg rule)

4 Results and Discussion

In this work, we calculated the depth (Range) of Bragg peak in a medium of liquid water for an incident proton beam covering the energy range of *1-300 MeV*. We restricted our calculations of the loss of incident energy at each interaction of proton with water molecule to the physical processes. We used different semi-empirical models encompassed in a new algorithm model based on *C/C++*. We calculated the electronic and the nuclear energy loss per path length for complete physical processes contributing to the position of Bragg peak. The results are partly showed in Figures (1-6). We also calculated the stopping power for proton in liquid water by dividing the irradiated medium into several layers (Eqs. 26 -27). The thickness of each layer is taken randomly to be equal to the flight distance between two successive collisions. It is directly related to the incident proton collision mean free path, which is itself connected to the total interaction cross section. We therefore calculated the deposited energy of proton beam in liquid water as a function of the depth by appealing the different programs of cross sections and stopping cross sections to calculate the stopping power and to determine the range. Several Monte Carlo platforms and applications are available to be used for an analytical approximation of the range calculation of proton beam. In this work, we studied the interaction of proton beam with liquid water using Monte Carlo method like GEANT4-DNA, SRIM, and DOSIMEX platforms. We focused our work on the calculation of the range-depth of Bragg peak as a function of incident energy from 1 to 300 MeV. In table 1 are presented the results obtained from Monte Carlo method compared to the analytic ones from our method and the published data from ICRU-49 [4]. We notice that our results are in good agreement with the others from Monte-Carlo method and ICRU-49 data.

Table 1: *The range of proton calculated by ICRU, GEANT4, SRIM, DOSIMEX and Our analytical Program.*

	Range (cm) With:				
Energy (Mev)	ICRU	GEANT4	SRIM	DOSIMEX	Our work
1	0.002	---	0.0025	0.00197	0.0022
3	0.014	0.0139	0.0147	0.01400	0.0140
10	0.123	0.1173	0.1230	0.11700	0.1210
30	0.885	0.8790	0.8810	0.88900	0.8520
50	2.227	2.2270	2.2060	2.24600	2.1670
60	3.083	3.0730	3.0330	3.12900	3.1010
70	4.080	4.0530	4.0090	4.12200	4.0020
80	5.184	5.1380	5.0117	5.23300	5.0980
90	6.398	6.3590	6.3160	6.46000	6.3090
100	7.718	7.6910	7.5380	7.79100	7.6050
150	15.77	15.825	15.445	15.8480	15.739
175	20.62	20.652	20.187	20.2880	20.649
200	25.96	26.025	25.451	26.1360	26.087
300	51.45	51.317	50.877	52.2360	52.055

We used these data from different methods to study the behavior of Bragg peak range as a function of incident energy. We show in Fig. 7 the relationship that could govern the loss of an incident energy E (MeV) or Bragg peak range R (cm) of a proton projectile in liquid water:

$$R = N \times E^{\beta} \qquad (31)$$

Where N is the proportionality factor and is approximately proportional to the square root of the effective atomic mass of the medium, $\sqrt{A_{eff}}$. The parameter β is an exponent factor of the incident energy.

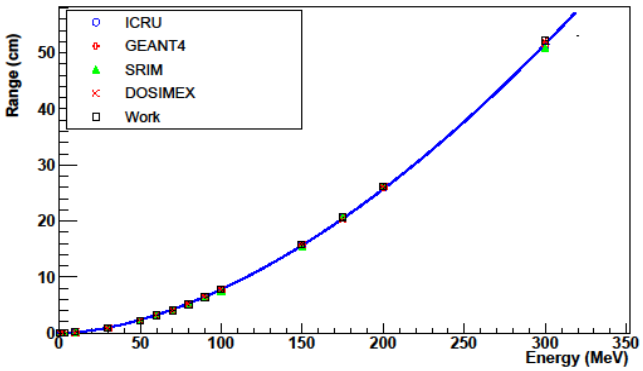

Fig 7: Range-energy relationship comparison between: ICRU, GEANT4, SRIM, DOSIMEX and Our analytical Program

In table 2, we show the values of both parameters N and β obtained from the fit of different data from our analytic method, Monte-Carlo method and ICRU data. They are in good agreement with the well-known and empirical Bragg-Kleeman rule [16, 22].

TABLE 2: *VALUE OF THE FIT PARAMETERS OF BRAGG-KLEEMAN RULE*

	N(g/cm²MeV)	β (dimensionless)
ICRU data	0.0023	1.75
GEANT4	0.0025	1.76
SRIM	0.0020	1.79
DOSIMEX	0.0024	1.75
Our Work	0.0021	1.77

We also developed, as showed in Fig. 8, a power expansion of the range-energy relationship. We get a polynomial formula of fourth degree as follow:

$$R = \sum_{n=0}^{N} a_n E_0^n \qquad (32)$$

In table 3 are displayed the values of parameters a_n compiled from different data of GEANT4, DOSIMEX, SRIM and ICRU. For convenience the new parameters are compared to the ones obtained by Ulmer et al [25].

TABLE 3: VALUES OF THE FIT PARAMETERS FOR THE FOURTH DEGREE POLYNOMIAL.

	a_1	a_2	a_3	a_4
ICRU data	4.98e-03	8.64e-04	-1.64e-06	2.19 e-09
GEANT4	5.71e-03	8.17e-04	-1.08e-06	5.38 e-10
SRIM	6.59e-03	8.21e-04	-1.62e-06	3.11 e-09
DOSIMEX	-1.32e-03	1.09e-03	-3.83e-06	8.31 e-09
Ulmer's coefficient	6.94e-03	8.13e-04	-1.21e-06	1.05 e-09
Our Work	5.20e-03	8.32e-04	1.38e-06	1.75 e-09

The new relationship between the incident energy E and the traversed range R investigated in this work for an incident proton beam in a medium of liquid water could be efficiently used for further complicated medium since the experimental data of reaction cross sections and range are not always available for deeply studies. For the latter case, we could extrapolate the range of each medium from the one measured for liquid water by using the Bragg-Kleeman rule. However, we used in this work the new formula (Eq. 31) to calculate the residual energy at each impact step of proton beam with water molecules. Along the z direction of incident beam, the remaining energy E(x) is calculated as a function of the maximum depth R_0 :

$$E(x) = \frac{1}{\sqrt[\beta]{N}} \sqrt[\beta]{R_0 - x} \qquad (33)$$

And, the linear stopping power could be obtained from:

$$S(x) = -\frac{dE}{dx} = \frac{1}{\sqrt[\beta]{N}} \sqrt[\beta]{(R_0 - x)^{1-\beta}} \qquad (34)$$

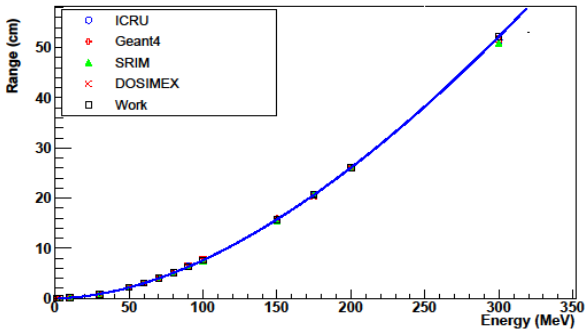

Fig 8: Range-energy relationship comparison between: ICRU, GEANT4, SRIM, DOSIMEX and Our analytical Program.

In Fig. 9 are presented the calculated E(x) and S(x) for an incident proton beam, with energy of 300 MeV, in liquid water. The figure shows the evolution of linear stopping power along the track x as a function of residual energy E(x). It starts to be small, only sensitive to the ionization processes, till the end of track where the loss of energy is dominated by the charge exchange and excitation processes.

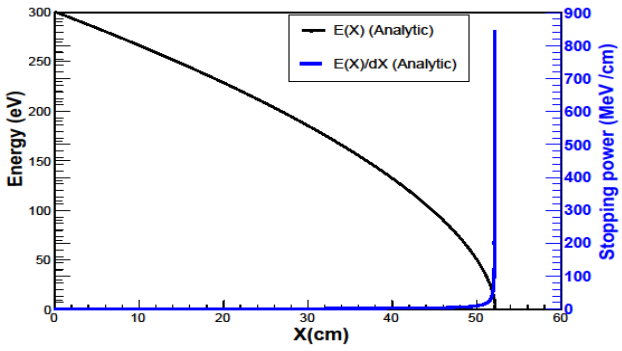

Fig 9: The analytic calculation of E(x) and dE(x) / dx as a function of X = Range (cm) by using eq. (33) and (34)

5 CONCLUSION

In this work, we presented an analytical method for the range calculation of protons beam, with incident energy of 1 – 300 MeV, in a medium of liquid water. We showed the role of various physical processes to improve the depth of the Bragg peak. We investigated the inelastic and elastic interactions for calculation of the cross sections and the stopping power. The obtained results showed to be in good agreement with the compiled data from ICRU (1993). We also investigated the nuclear stopping power; even its effect is less than 5% at low energy according to the electronic one. We quantified the contribution of nuclear effect on the range depth as a function of the incident energy. We studied the relationship between the range of Bragg peak and incident energy of proton beam in water liquid. We proposed a new parameterization of range, known as Bragg-Kleeman rule, from a set of compiled data from GEANT4, SRIM, DOSIMEX and ICRU (1993). For further study, we could use this new formula to calculate the loss of energy and the linear stopping power of more complex medium like DNA.

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