MONTE CARLO COMPUTATION OF THE ENERGY DEPOSITED BY HEAVY CHARGED PARTICLES IN SOFT AND HARD TISSUES

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Înţelegerea în detaliu a fenomenelor nucleare care apar la bombardamentul ţesuturilor biologice cu ioni de energie mare conduce la o problemă dificilă de fizică nucleară datorită complexităţii ţintei şi a mecanismelor de reacţie implicate. Rezolvarea acestei probleme are o relevanţă deosebită pentru modernizarea tehnicilor de hadrono-terapie în medicină şi a radioprotecţiei fiinţelor umane în călătoriile cosmice. În acest studiu prezentăm un ansamblu de simulări Monte Carlo pentru interacţia unor particule încărcate grele având potenţiale utilizări medicale, cu ţinte de apă şi calciu. Am ales aceste ţinte ca modele primare a ţesuturilor biologice moi şi dure. Instrumentul de calcul utilizat în simulări a fost codul FLUKA.

Understanding in details the nuclear phenomena appearing at the bombardment of the biological tissues with high energy ions poses a challenging problem for nuclear physics due to the complexity of the target and reaction mechanisms involved. Solving this problem has a significant relevance for the refinements of the hadron-therapy techniques in medicine and radioprotection of humans in space travels. In the present study we develop complex numerical Monte Carlo simulations for the interaction of high energy heavy charged particles of potential medical interest with water and calcium targets. We choose these targets as rough models for soft and hard biological tissues, respectively. The computational tool employed in the simulations was FLUKA computer code.

Keywords: Charged hadrons interactions, energy deposition, Bragg curve, Monte Carlo simulations, hadron-therapy

1. Introduction

In the process of slowing down of charged ions in matter the energy loss occurs dominantly via inelastic collisions with atomic electrons [1]. Slower particles give more energy to the electrons in comparison with faster particles, therefore, the delivered dose increases with penetration depth up to a sharp maximum at the end of the particle trajectory. This is the Bragg peak, named after

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William Bragg, who observed for the first time an increase of the ionization density at the end of the range of alpha particles in air [2]. The entire depth-dose distribution is usually called Bragg Curve. For the heavy charged particles the highest radiation dose is delivered to the region of the target near the points where the particles stop, while the dose elsewhere in the target is low.

The amount of average energy deposition and their position in media like tissues is so important because it makes un-repairable tissue in desire position and giving fewer doses to surrounding area. The occurrence of the Bragg peak makes heavy charged beams useful tools for treatment of the deep-seated tumors in living organisms. The advantages of proton and heavy ion therapy (so called *hadron-therapy*) over the conventional photon and electron therapies are due to the better physical dose distributions achievable by inversed dose profile at the end of their range, tumor-conform treatment, and the radiobiological characteristics of heavy ions [3]. The promoter of the hadron-therapy was Robert Wilson [4] who realized for the first time that high energy beams of protons and heavy ions offers the “magic bullet” able to irradiate deep seated tumors in organisms with a minimum irradiation of the penetrated healthy tissues. Only in the last decade this techniques gain high social interest due to the advances in high energy beams technology [5] which increase the precision of dose deposition and conduct to socially-affordable costs to be applied at large scale in medical clinics [6].

In order to reach the Bragg peak position around 20 cm depth in a biological tissue the energies needed are typical 150-200 MeV for proton and 3500-4000 MeV for carbon ions beams. Biological matter is a complex “target” made of several tens of medium-heavy mass isotopes. In the slowing down process the ions energy ranges all values down to keV close to the end of the trajectory. Although the dominant processes in the energy transfer from the beam to the stopping medium are atomic in their nature, a considerable amount of residual radioactivity is produced by nuclear reactions. In order to be able to design an accurate treatment planning it is important to obtain precise estimates for the induced radioactivity and their evolution in time. This is a tremendous problem for nuclear physics, implying cascades of atomic and nuclear processes at energies from hundreds of MeV per nucleon to near zero and a target composed of tens of isotopes [7]. The experimental knowledge is very limited, therefore high accuracy numerical simulations are crucial in studying this complex problem.

It is the goal of the present work to report new numerical Monte Carlo simulation for the interaction of protons and heavy ions with biological-like materials concentrating on the energy losses by atomic processes. In a forthcoming paper this study will be continuated with the focus on the nuclear interactions. We selected simple models for the soft and hard biological tissues as water and natural calcium targets, respectively. Although by making this choice we do not expect to obtain accurate predictions of the induced radioactivity in real organisms, the Bragg peak position can be predicted with accuracies of few percents. Following a set of simulations for all types of radiations currently employed in radiotherapy, detailed calculations are presented for stopping of heavy ions from ^{7}Li to ^{56}Fe in H_2O and $^{nat.}Ca$ targets. Comparisons with experimental data are made whenever these are available. The instrument used in our simulations is the computer code FLUKA [8] developed at CERN and Milano.

2. Energy loss by charged particles and photons in matter

Monte Carlo simulation techniques implemented in the FLUKA computer code allows numerical simulations for charged hadronic beams (protons, deuterons, alphas and Heavy Ions), electrons and photons. In order to obtain a comparative picture of the energy depositions by these radiations in materials we performed calculations of the average specific energy deposition (a quantity proportional with the dose) in a 20 cm thick water target as a function of the penetration depth. A number of 100000 Monte Carlo "histories" have been done for each type of radiations in order to reduce the variance and keep a reasonable computer time. The results of these calculations are presented in fig. 1.

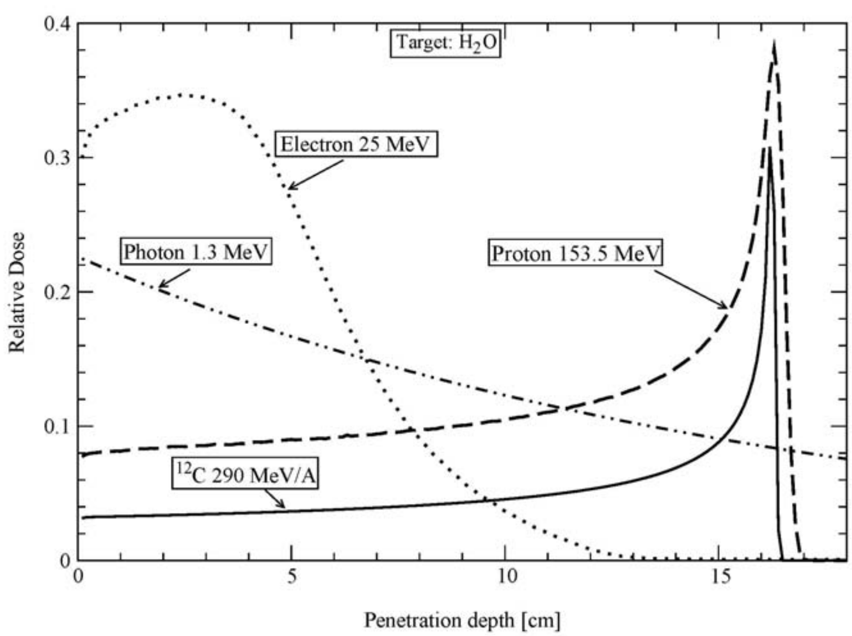

Fig. 1. Relative dose deposited in a thick target of water as a function of the penetration depth by several types of radiations employed in radiotherapy. The simulations have been performed with the computer code FLUKA.

A typical photon beam used in radiotherapy contains gamma photons of *1.3 MeV* which is produced by a ^{60}Co radioactive source (cobalto- therapy). As shown in Figure1 (dot-dashed line) this beam transfers to the water environment a dose with a rate that decays almost linearly from the entrance surface to the end of the trajectory. Our calculations indicate that near the surface the average energy density deposited (proportional with the dose) is $<\rho> \approx 0.22\ GeV/cm^3$ and decreases to $<\rho> \approx 0.08\ GeV/cm^3$ at *18 cm* depth in water. Therefore, in order to deposit a unit of energy in a cubic centimeter of material located at *18 cm* depth via a *1.3 MeV* photonic beam the same volume of material located near the entrance surface has to receive a quantity of energy *2.76* times higher. Moreover, as can be seen from Figure 1, the photons beam penetrate much deeper in the target deposing significant energy at depths higher than one of interest.

Calculations performed for *25 MeV* electrons (dotted line in Figure 1) shows that the incident beam will depose energy in the water target up to a depth of *15 cm*. A maximum will occur at about *3 cm* followed by a continuous decrease, in the range from *4* to *13 cm*, the average energy density decreasing from *0.9* to *0.1* from its maximum. The maximum transferred dose will occur below the entrance surface at *3-4 cm* depth then it shows up a gradually decrease to the depth of about *13 cm*. Therefore, as can be observed from Figure 1, if the goal is to irradiate a volume of the target located e.g. at *16 cm* depth by using photons or electrons, a significantly higher irradiations will occur in the entry region before the point of interest. In the view of practical medical applications, conventional beam radiotherapy with photons and electrons is limited because healthy tissues are also irradiated during treatment. A significant improvement in this problem can be obtained by focusing on the tumor several very low intensity beams from different directions ("gamma knifes" for photons) [9].

In the case of stopping hadronic beams we choose as examples proton and carbon ions with energies of *153.5 MeV* and *290 MeV/A* respectively in order to locate the Bragg peak positions at *16.3 cm* depth where we assumed to be located the target volume (tumor in medical applications). As can be seen from the Figure 1 the ratio of the Bragg peak dose versus dose in the entrance region is *2.3* times larger for carbon than for protons. Because of their larger mass, also the angular and energy beam straggling becomes negligible for carbon as compared with protons [10]. These observations indicate that the carbon beams have better physical characteristics than protons in view of the radiotherapy applications. In addition, carbon exhibits a strong increase of the Linear Energy Transfer (LET) in the Bragg peak as compared with the entrance region. Nowadays a large variety of heavy ion beams with energies of hundred *MeV/A* are available at research facilities [11]. Their potential use for hadrontherapy is still under investigation.

We developed in the present study detailed stopping Monte Carlo simulations in water and calcium thick targets, selected as simple models for soft and hard biological tissues respectively. The calculations were performed for 8 heavy ions between Li and Fe.

3. Stopping of heavy charged particles in condensed matter

As discussed before, in order to penetrate tens of cm in biological tissues charged heavy ion beams need the entrance energies of the order *200 MeV/A*. For energies between ≈ *0.5 MeV/A* and *200 MeV/A* the atoms in the stopping medium can be excited or ionized. These processes are electromagnetic by their nature and are well understood leading to the stopping power that can be calculated analitically. The energy loss (S_l) as function of particle energy and atomic number is given by the Bethe-Bloch-formula [12, 13, 14, 15]:

$$|S_l| \equiv \frac{dE}{dx} = \frac{4\pi Z_{eff}^2 e^4 n_e}{m_e v^2} \ln\left[\frac{2mv^2}{\langle I\rangle(1-\beta^2)}\right] + \text{(higher relativistic terms)} \quad (1)$$

where n_e is the density of the electrons of the target material, e the elementary electric charge, m_e is the electron mass, v the particle velocity, β is the particle velocity in units of velocity of light, m the mass of projectile and $<I>$ the mean ionization potential of the atoms in the stopping medium. Z_{eff} is the effective charge empirically approximated by Barkas [16]. At high energies, all projectile are stripped off their electrons and the effective charge equals the atomic number. At small energies (close to the end of the trajectory – Bragg peak region) electrons are collected from the target atoms and the effective charge of the projectile decreases, becoming closed to zero when the particles stop. The change of Z_{eff} is the main reason for the sharp decrease of the energy loss at lower energies, which is the essential criterion for the use of heavy particles in therapy. The average ionisation potential $<I>$ is the average value of the excitation energies over all atomic states weighted by their transfer probability to continuum. These probabilities, which are approximated as *optical dipole oscillator strengths*, are unknown for most material other than hydrogen. When one deals with a compound medium, which is the case in hadron-therapy, it is possible to use the *Bragg's rule*: the S_l value for compound can be found by averaging the S_l over each atomic element in the compound weighted by the fraction of electrons belonging to each element. In Eq.(1) the electron density of the material can be calculated with the relation:

$$n_e = \frac{N_A \cdot Z \cdot \rho}{A} \quad (2)$$

where ρ is the density of the material, Z, A the atomic number and mass number, respectively, and N_A the Avogadro number. For low energies, i.e. for small (compared to the speed of light c) velocities of the particle (β<<1), the energy loss according to formula (1) decreases approximately as $1/v^2$ with increasing energy and reaches a minimum for about $E = 3mc^2$, where m is the mass of the incident particle. For highly relativistic cases ($\beta \approx 1$), the energy loss increases logarithmically due to the emission of electromagnetic radiation by bremsstrahlung.

The range of the incident particles R in a stopping medium can be determined by integrating the stopping power S_l from values close to zero (at the end of the trajectory) to E_0 (the incident energy):

$$R = \int_0^{E_0} \left| \left(\frac{dE}{dx} \right) \right|^{-1} dE \tag{3}$$

a relation valid in the so called *continuous slowing down approximation (CSDA)* [15]. In practice, however not all particles that start with the same energy will have the same range. This is caused by the statistical fluctuation in the energy loss process. For a given ion it is possible to fit the relation between R (in g/cm^2) given by Eq. (3) and the incident energy E_0 (in MeV) for a particle of mass M by the Bragg-Kleeman rule [17] which in the relativistic and *CSDA* approximations has the form :

$$R = a \cdot \left(E_0 + E_0^2 / 2MC^2 \right)^p \tag{4}$$

where factor a is approximately proportional to the square root of the effective atomic mass of the stopping medium and p is a phenomenological energy-dependent parameter.

The above formalism based on analytical formulas gives a rough estimation of the energy deposition by heavy ions in matter and can be used to estimates the Bragg peak position. A different approach, much more powerful is based on a Monte Carlo approach, simulating the history of each individual particle of the beam from the entrance point of the target material up to the end of its trajectory. By this technique it is possible to go beyond the average values, estimating doses in any volume of arbitrary shape from the target material. We employed in our study this numerical simulation procedure, implemented in the FLUKA computer code [8]. FLUKA (FLUktuierende KAscade*)* is a Monte Carlo code able to simulate transport and interaction of electromagnetic and hadronic particles in any target material over a wide energy range. It is a multi-purpose, multi-particle code that can be applied in many different fields. In FLUKA "continuous" processes such as energy loss and angular deflections due to Coulomb interactions and "discrete" (or "explicit") processes (delta-ray production, nuclear interactions, decays, bremsstrahlung and photon interaction) are treated separately.

We considered as a test case for our computation procedure a beam of ^{12}C ions with *290 MeV/A* energy bombarding a thick water target. Experimental data on the Bragg peak position for this case were taken from ref. [18]. A comparison of the Bragg peak position obtained by our calculations and the experimental results is presented in fig. 2. A reasonable agreement with the experiment (precisions of *1-2 mm*) was obtained by our simulations, as long as it was not the purpose in the present stage to perform a fine tuning of the input parameters employed in the FLUKA calculations.

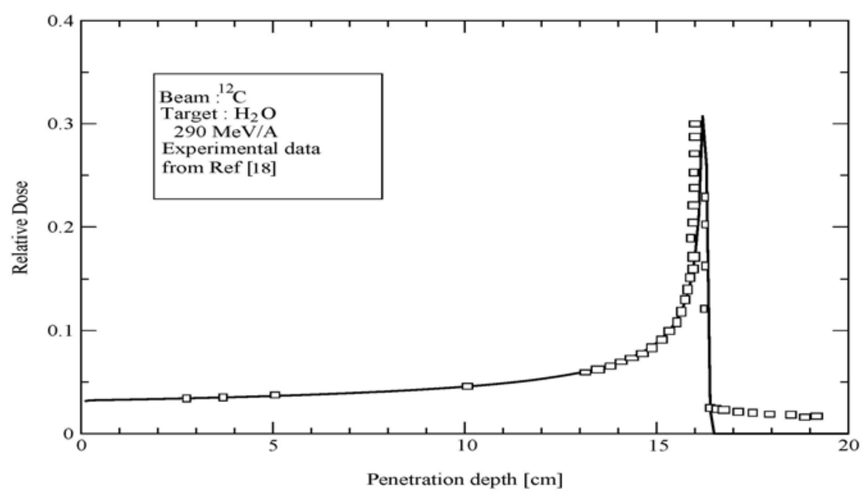

Fig. 2. Comparison between experimental data and our calculations for the average density of the deposited energy of ^{12}C ions stopped in water. Note that at depths between 16 and 19.5 cm it can be observed in the experimental data fragmentation products, not described by the present numerical simulations.

As can be observed from fig. 2 the experimental data shows a tail on the right-hand side of the Bragg peak, which is not reproduced by the present calculations. This tail is produced by the beam fragmentation products and its description can be obtained only by taking into account in details the nuclear processes, a goal beyond the purposes of the present paper.

4. Stopping of heavy ions in water targets

The simplest model for the biological soft tissues can be obtained by choosing a water target. In these calculations at a reasonable computation time, we considered *100000* of particles histories in the Monte Carlo simulations. Each history begins with a *150 MeV/A* at normal incidence on a parallelepiped target. Particle transport threshold was set at *100 keV* in the FLUKA input data. By successive interactions of the incident particles with atomic electrons and nuclear collisions the energy is reduced gradually and below of threshold the histories are completed. For comparison between different heavy charged particles interactions with water, we calculated average energy deposition (relative dose) by heavy ions from ^{7}Li to ^{56}Fe with the same energy per nucleon *(150 MeV/A*). Our Monte Carlo simulations conducted to the Bragg curves shown in Figure 3. Form this Figure can be observed that ^{7}Li penetrates about *10 cm* in water while carbon and iron can penetrate *4.5* and *1 cm*, respectively. Therefore for reaching *10 cm* depths in water with ^{56}Fe ions the incident energy should be more than *8400 MeV.* The ratio of the Bragg Peak dose to the entrance dose for nitrogen and carbon are similar but the penetration depth is *3.5* and *4.5 cm*, respectively.

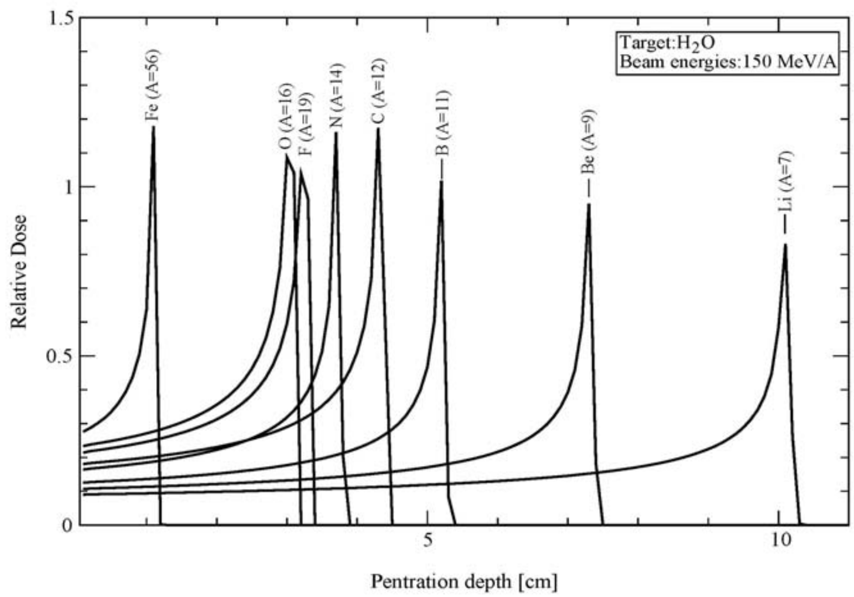

Fig. 3. Average energy density deposited by heavy ion beams in a thick water target as a function of the penetration depth obtains by numerical Monte Carlo simulations with FLUKA code.

Bragg-Kleeman relation (Equation 2) gives in the first approximation a rough linear dependence of the particles range *R* on their incident energy E_0. We aimed in our numerical study to obtain a precise dependence of the particles Ranges at a given energy per nucleon. Precise values for ranges, obtained by our Monte Carlo calculations are presented in Fig. 4, for different ions with the same kinetic energy per nucleon (*150MeV/A*). At the same kinetic energy per nucleon, lighter particles move faster, spending in average less time near outer atomic electrons. This reduces the effect of Coulomb interactions (hence stopping power) and increases range. As shown in fig. 4, the ranges change abruptly between proton and oxygen ions, and then a quasi-linear decrease can be observed between ^{28}Si to ^{56}Fe ions.

At *150 MeV/A* protons penetrate about *15.5 cm* in water, oxygen ions *4.2 cm* and Iron *2.7 cm*. The results presented in fig.4 indicate the limitation of Equation (3) in obtaining the range values for different heavy ions. For practical applications an accurate numerical simulation has to perform in each case.

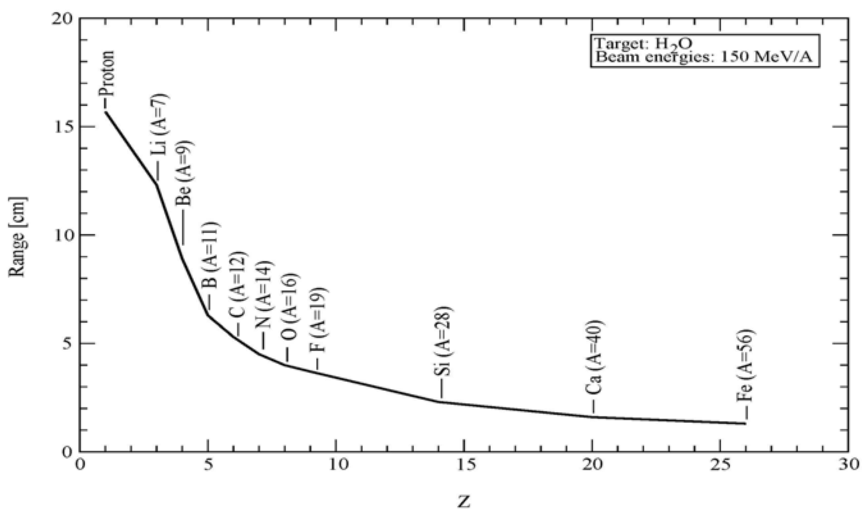

Fig. 4. The evolution of the Bragg peak position (average range) at stopping in water of different heavy ions with 150 MeV/A incident energies.

5. Stopping of heavy ions in calcium targets

A simple model for biological hard tissues (bones) can be obtained by considering a natural Calcium target ($^{nat.}Ca$). Bragg curves obtained by FLUKA simulations for *9* heavy ions between *Li* and *Ca* are shown in Figure 5. The energy per nucleon was kept constant at *150 MeV/A* as we did in the study of the water target.

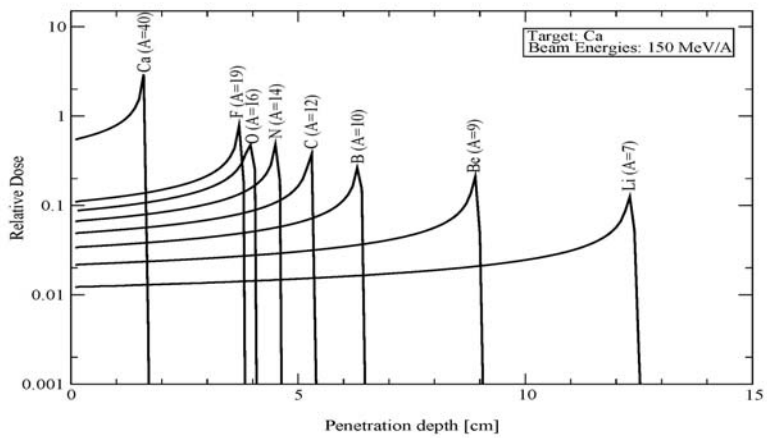

Fig. 5. Average energy density deposited by heavy ions beams in a thick ^{nat}Ca target as a function of the penetration depth obtained by numerical Monte Carlo simulations with FLUKA computer code.

As shown in fig. 5 at the same energy per nucleon, ^{7}Li and ^{40}Ca can penetrate in a calcium targer *12.4* and *1.6 cm* respectively. If the application needs penetration depth of *12.4 cm* for a ^{40}Ca beam its energy must be greater than *46 GeV*. For the projectiles with intermediate *Z* values such as carbon and nitrogen the penetration depths are *5.1* and *4.2 cm* respectively. Deviations from the Bethe-Bloch formula predictions of ranges, obtained by our Monte Carlo simulations are shown in fig. 6 for the ^{nat}Ca target.

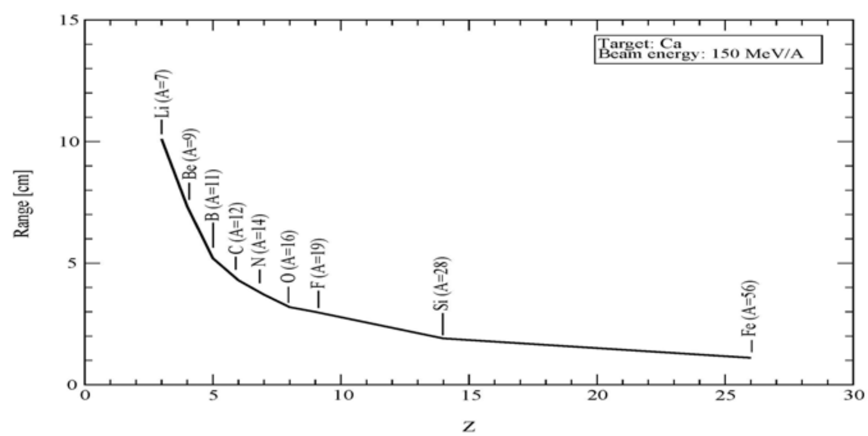

Fig. 6. The evolution of the Bragg peak position (average range) at stopping in $^{nat.}$Ca thick target of different heavy ions with 150 MeV/A incident energies.

As expected, penetration depths of heavy charged particles in calcium targets are smaller than in water. From Figure 6 can be observed that at *150 MeV/A* incident energy the penetration depth decrease fast with about 30% for ions between Lithium and Fluorine (*6* units in *Z*), then a shallow decrease between Fluorine and Iron (*17* units in *Z*). Aside their absolute values, the curves from Figures 4 and 6 have similar shapes. A notable difference between our primitive models of soft and hard biological tissues appears when we consider the nuclear reactions when different channels appear on each energy interval. The present calculations offer also guidance for selecting the proper reaction mechanisms appearing at different depths in the target. This important issue will be approached in a forthcoming work.

6. Conclusions

In the present work we employed Monte Carlo calculations in order to compute Bragg curves and ranges for two simple models of the soft and hard biological tissues – water and calcium targets respectively. The calculations were performed for incident projectiles between protons and iron ions at *150 MeV/A* Ienergy. The simulations have been performed with the computer code FLUKA, a tool designed mainly for high energy basic research. Our results show that this code can be used as a reliable instrument for estimating the deposed dose and treatment planning in hadrontherapy. An inspection of the literature shows that the experimental data on the heavy ions stopping power are very scarce in the energy domain investigated in the present study. It is therefore necessary to rely completely on theoretical estimations as those presented in this work.

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