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Lateral spread of dose distribution by therapeutic proton beams in liquid water

Isabel Abril^{a,*}, Pablo de Vera^a, Rafael Garcia-Molina^b, Joanna Kyriakou^c, Dimitris Emfietzoglou^c

^a Departament de Física Aplicada, Universitat d'Alacant, E-03080 Alacant, Spain

^b Departamento de Física – Centro de Investigación en Óptica y Nanofísica, Regional Campus of International Excellence “Campus Mare Nostrum”, Universidad de Murcia, E-30100 Murcia, Spain

^c Medical Physics Laboratory, University of Ioannina Medical School, GR-45110 Ioannina, Greece

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ABSTRACT

We have calculated the lateral spread of the dose distribution of protons in liquid water by means of the SEICS (Simulation of Energetic Ions and Clusters through Solids) code, which properly accounts for the electronic stopping force (including energy-loss straggling), multiple elastic scattering with the target nuclei, dynamical electron charge-exchange processes and nuclear fragmentation reactions between the projectile and the nuclei of the target. Due to the multiple elastic scattering processes part of the proton energy may be deposited at a given lateral distance from the initial beam direction, which is quantified by the root mean square radius (r_{rms}). We find in our simulations that the r_{rms} follows a parabolic dependence as a function of the depth in the target and the quotient between r_{rms} at the Bragg peak and the depth of the Bragg peak is around 3% independently of the proton energy. A rather good agreement is obtained when comparing our results of r_{rms} with experimental data and with other models.

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1. Introduction

Radiotherapy using high-energy ion beams (also called hadron therapy) is one of the most promising techniques for those cancer treatments where high precision is required. It is becoming increasingly popular due to the precise way in which energetic ions deliver their energy into the tumor area. This method offers significant advantages compared with conventional photon or electron therapy, because it exhibits a superior ability to conform the dose distributions to cancer volumes while the exposure of the healthy surrounding tissues can be drastically reduced, which in turn may result in a better local control of the disease and patient survival [1–3].

In contrast to the depth-dose profile of photons and electrons, the energy deposition pattern of ions is characterized by a low-dose plateau at the entrance region, followed by a sharp dose increase near the end of the ion range (the so-called Bragg peak) and a well-defined fall-off with almost zero dose behind that peak. Therefore, the possibility of delivering large and uniform dose distributions makes of ion beams a suitable technique for external

radiation therapy in which the preservation of organs proximal to the target and the sparing of critical structures distal to the target are crucial [4].

In order to achieve high precision in hadron therapy treatment planning, a fundamental requisite is to predict with accuracy the ion depth-dose curves, as well as its radial distribution with respect to the incident beam direction. Therefore, it is necessary a precise description of the interaction of the incident projectile beam with biological targets, which will lead to a better three-dimensional characterization of the dose distributions in the patient's organs. Among the type of particles used in hadron therapy, the most utilized are proton and carbon ion beams; in this work we will concentrate in proton beam cancer therapy.

The evaluation of proton depth-dose distributions can be obtained by analytical methods or by Monte Carlo techniques. Several analytical and semi-analytical models have been proposed to calculate the dose delivered in different biomaterials. These depth-dose calculation algorithms have widely been used because of their simplicity and short calculation time [5–7], two relevant features for fast assessment of dose distribution and biological effects in treatment planning. However, these analytical calculations do not always agree well with the measurement results, since they make a series of assumptions in order to simplify the calculations [8]. On the other hand, Monte Carlo simulations are com-

* Corresponding author. Tel.: +34 965909578; fax: +34 965909726.

E-mail address: ias@ua.es (I. Abril).

monly accepted as the most precise way to compute the proton dose distributions in complex materials such as tissues of the human body. This is because Monte Carlo methods can take into account the physics of particle interactions with the target constituents on an event-by-event basis using theoretical models or experimental cross-section data for electromagnetic and nuclear interactions, but in contrast they become very time consuming and are difficult to use for routine treatment planning. Several Monte Carlo approaches have been proposed, such as SHIELD-HIT [9], PHITS [10], GEANT4 [11], FLUKA [12], KURBUC [13] or MCHIT [14]. Monte Carlo calculations prove that proton dose distribution not only depends on electromagnetic interactions with target electrons, but also on nuclear interactions, such as fragmentation reactions and multiple scattering interactions [14–16].

The aim of this work is to obtain accurate three-dimensional proton depth-dose distributions by a detailed and realistic treatment of the main processes between the incoming projectile and the biological target. For that purpose we use the simulation code SEICS (Simulation of Energetic Ions and Clusters through Solids) [17,18] based on Molecular Dynamics and Monte Carlo techniques to follow the trajectory of the projectiles through the target. The main features of this code are outlined in Section 2. In our study, monoenergetic proton pencil beams at therapeutic energies (up to 250 MeV) traveling in liquid water, a common surrogate of living tissues, are considered. The electronic stopping power and the energy-loss straggling are accounted for realistically by using the MELF-GOS methodology [19,20], which is based on a proper description of the experimental electronic excitation spectrum of the target. With the SEICS code we can map the energy deposited in the target by the projectiles, both in the longitudinal and transverse directions of the incident beam. In Section 3 we present results of the root mean square radius (r_{msr}) of the proton beam as a function of the depth in the target, which characterizes its lateral dispersion due mainly to multiple elastic scattering with the target nuclei. We find that the r_{msr} has a parabolic dependence with the depth z in the target, and that its value at the Bragg peak depth is always around 3% of this depth, irrespectively of the proton initial energy. For liquid water we obtain a simple dependence with the incoming proton energy of the parameters entering in the quadratic dependence of the r_{msr} with the depth. Our calculations of the spread of the incoming proton beam with the depth are compared with experimental data, resulting in a rather good agreement. Finally, the conclusions of this work are summarized in Section 4.

2. Simulation procedure

Consider a pencil proton beam consisting of monoenergetic particles, at energies of therapeutic interest around several hundred of MeV, that initially travel in the z direction along a liquid water target. The incoming charged particles undergo electronic, atomic and nuclear interactions. The dose delivered by the proton beam in the biological medium is simulated by the SEICS code, which follows in detail the trajectories of the protons in the target by solving their equation of motion through a modification of the Verlet's algorithm to account for the relativistic velocity of the projectile [17,18]. Therefore, when the projectile has an instantaneous position $\vec{r}(t)$ and velocity $\vec{v}(t)$, and the force that acts on it is $\vec{F}(t)$, the projectile's new position $\vec{r}(t + \Delta t)$ and velocity $\vec{v}(t + \Delta t)$ after a time step Δt are given by the following expressions:

$$\vec{r}(t + \Delta t) = \vec{r}(t) + \vec{v}(t)\Delta t + \frac{\vec{F}(t)}{2M}(\Delta t)^2[1 - (v(t)/c)^2]^{3/2}, \quad (1)$$

$$\vec{v}(t + \Delta t) = \vec{v}(t) + \frac{\vec{F}(t) + \vec{F}(t + \Delta t)}{2M}\Delta t[1 - (v(t)/c)^2]^{3/2}, \quad (2)$$

where M is the mass of the projectile and c is the speed of light. The force $\vec{F}(t)$ felt by the projectile is the electronic stopping force, which due to the stochastic nature of energy-loss interactions between it and the electrons of the medium is accounted for by a Gaussian distribution centered in the stopping power S with a variance depending on the energy-loss straggling Ω^2 , $\sigma^2 = \Omega^2/(\nu\Delta t)$. A Monte Carlo method is applied to randomly sample the force according to the following expression:

$$\vec{F} = -\left[S + \frac{\Omega}{\sqrt{\nu\Delta t}}\sqrt{-2\ln\zeta_1}\cos(2\pi\zeta_2)\right]\hat{v} \quad (3)$$

where ζ_1 and ζ_2 are random numbers uniformly distributed between 0 and 1, and $\hat{v}$ is the unit vector of the instantaneous projectile velocity $\vec{v}$. The input data of the SEICS code are the electronic stopping power S and the energy-loss straggling Ω^2 , which depend on the projectile charge and velocity, as well as on the target electronic properties. These magnitudes are calculated within the dielectric formalism using a realistic electronic excitation spectrum of the target, which is evaluated by the MELF-GOS (Mermin Energy Loss Function-Generalized Oscillator Strength) model, where a fitting to the available optical experimental spectrum of the target is made [19,20]. The contribution of the projectile polarization due to the self-induced electric field in the target is also taken into account [21]. By using this methodology we obtain accurate values of S and Ω^2 , which agree very well for elemental and compound targets when compared with experimental data, especially for protons in liquid water [18,22]. The mean excitation energy of the target is also calculated within this model, giving a value of 79.4 eV [23], which is employed to compute the stopping power at high proton energies through the analytical relativistic Bethe formula [24]. Note that the main difference in the predictions of the Bragg curve at clinical proton energies lies in the value used for the mean excitation energy for water [25]. The dynamical electron capture and loss processes between the projectile and the target electrons, as well as their associated energy loss, are taken into account by a Monte Carlo procedure in the SEICS code, using the fractions of the charge states at the dynamical equilibrium [26].

The statistical nature of the multiple elastic scattering between the projectile and the target nuclei is included in the simulation through a Monte Carlo scheme, in such a manner that provides the projectile scattering angle and the corresponding elastic energy loss at each collision. The probability to decide the type of target atom that undergoes an elastic collision with the projectile is taken proportional to the fractional contribution made by each atom to the total collision cross section. The scattering between the projectile and the target atom is described by a Thomas-Fermi Coulomb screened potential with the universal screening length [27]. Elastic collisions with atomic nuclei involving large impact parameters are much more probable than small impact parameter collisions, therefore each proton will undergo a large number of elastic interactions, whose stochastic nature can adequately be accounted for by means of a Monte Carlo algorithm [28]. These processes are responsible of the change in the trajectory of the incoming ions as a result of angular deflections. Also, elastic scattering contributes to the energy loss at low energies.

The fragmentation reactions between the incoming proton and the target are also considered in the SEICS code to determine the depth-dose distribution. Our model considers the attenuation of the primary proton flux with the depth according to the ICRU data [29] for the total fragmentation nuclear cross sections, and a local energy deposition of a fraction of the residual energy of the secondary products. This approach is valid in the case of proton beams, where target fragments are generated with low energies, having an energy deposition close to the ion track and with small influence in the beam width [30]. The effects of nuclear

interactions are more pronounced with increasing proton energies, giving a decrease in the Bragg peak amplitude. At projectile energies of several hundred of MeV/u it is indispensable to include fragmentation reactions to obtain accurate values of the depth-dose distributions.

As stated in the previous paragraphs, the simulation code SEICS describes realistically all the interactions between the incoming projectile and the target, whose electronic excitation spectrum is properly taken into account by the MELF-GOS model. This procedure allows accurate simulations of the dose profile, the energy distribution and the widening of the beam as a function of the depth.

3. Results and discussion

When an initially monoenergetic proton pencil beam directed along the z-axis interacts with a biological target, a degradation of the proton energy occurs due mainly to inelastic collisions, and a broadening of the beam takes place due to the multiple elastic scattering. Therefore, knowledge of the Bragg curve is not sufficient, and three-dimensional dose distributions are necessary for accurate treatment planning in hadron therapy. Here we present results obtained with the simulation code SEICS regarding the dose distributions of pencil proton beams in liquid water, making special emphasis in their lateral spread due to multiple elastic scattering.

The three-dimensional distribution of deposited energy along the projectile track can be described through the lateral dose distribution $\Phi(z, r)$, i.e., the dose delivered in the target at each depth z and at a given radial distance r perpendicular to the projectile incident direction. Due to the azimuthal symmetry of the problem, the x and y directions are equivalent, therefore in order to visualize the lateral dispersion of the dose we use the function $\Phi(z, x) = \Phi(z) \frac{N(z, x)}{N(z)}$, where $\Phi(z)$ is the total dose at a given depth z , that is, the depth-dose curve. $N(z, x)$ represents the number of particles at a given depth z and at a given lateral distance x , with $N(z)$ being the total number of projectiles at a depth z . Note that $N(z)$ is not constant, since the number of projectiles in the beam decreases with the depth due to the stopping of particles and the fragmentation processes. In Fig. 1 we represent the lateral distribution of the deposited dose for a 200 MeV proton beam in liquid water obtained with the SEICS code. The larger concentration of deposited energy takes place along the beam entrance axis. However,

Fig. 1. Lateral distribution of the dose deposited in liquid water $\Phi(z, x)$ by a 200 MeV proton beam, as a function of the depth z and the lateral distance x from the initial beam direction.

due to multiple elastic scattering there is a lateral spreading of the energy deposited which grows as the depth increases and reaches its maximum value around the Bragg peak. Because of this spread, the lateral dose presents two maxima along the initial projectile direction (i.e., the z axis), one at the Bragg peak depth, where the depth-dose curve $\Phi(z)$ is maximum, and another one at the very beginning of the protons track, where all the particles are concentrated in a small region because negligible elastic scattering has occurred. Therefore, it is very important to take into account the multiple elastic scattering of the proton beam, since it gives a non-negligible lateral spreading around the Bragg peak, which leads to the degradation of the Bragg peak position prediction.

Since the lateral dose distribution depends directly on the radial distribution of particles along the beam path, it is very important to know the radial aperture of the beam, represented by the root mean square radius r_{rms} of the beam particles, $\langle r^2 \rangle^{1/2} = \sqrt{\langle x^2 \rangle + \langle y^2 \rangle}$, as a function of the depth z . As the SEICS code follows the trajectories of the protons through the target, it is possible to know their root mean square radius $\langle r^2 \rangle^{1/2}$, which indicates how much the incident particles scatter in a material.

In Fig. 2 we show by solid lines $\langle r^2 \rangle^{1/2}$ for protons in liquid water as a function of the depth z at energies of 180 and 215 MeV. A detailed comparison of our results with experimental data (symbols) [1] as well as with an analytical model (dashed line) [30] shows a rather good agreement. The discrepancies appearing at 215 MeV between the experimental data and the theoretical and simulated results at large depths can be understood because the energies used in the calculations were estimated from experiments [1] using the maximum ion range [30]. Also, the propagation of long-range secondary particles emerging from nuclear fragmentation reactions could contribute to the experimental lateral spread at large ranges.

It should be noted that, although the r_{rms} depends on the path traversed in the medium, on the atomic weight of the target and on the charge and energy of the incident projectiles, our simulations find that the quotient between the r_{rms} at the Bragg peak depth, $\langle r^2 \rangle_{\text{Bragg peak}}^{1/2}$, and the Bragg peak depth, $z_{\text{Bragg peak}}$, is always

Fig. 2. Root mean square radius $\langle r^2 \rangle^{1/2}$ of a proton beam in liquid water, as a function of the depth, at incident energies of (a) 180 MeV and (b) 215 MeV. The solid lines correspond to the results obtained with the SEICS code. A comparison with experimental data [1] (symbols) and with an analytical model [30] (dashed lines) is presented.

around 3%, independently of the initial proton energy, in the range from 5 to 250 MeV. For example, for a typical proton beam of 100 MeV used in hadron therapy, the spread of the beam at the Bragg peak is around 2 mm, whereas at 200 MeV it increases until around 7 mm.

In the same proton energy range (5–250 MeV), our simulations predict that $\langle r^2 \rangle^{1/2}$ increases with the depth following a parabolic dependence and suddenly falls down at the distal part of the Bragg peak. This behavior is due to the fact that only a few projectiles travel in almost straight line to reach these deeper regions, whereas most of the projectiles, that undergo multiple elastic collisions, deviate from their initial direction and stop at lower depths [31]. As the simulation of the radial dose distribution for each proton energy is very time consuming, it should be desirable to have an approximate analytical expression to provide the lateral spreading of the beam as a function of the depth. We have found that the root mean square radius $\langle r^2 \rangle^{1/2}$ of the beam as a function of the depth z is reasonably well fitted by the parabolic function.

$$\langle r^2 \rangle^{1/2} = C_1 z + C_2 z^2. \quad (4)$$

The coefficients C_1 and C_2 are obtained from simulations at several proton energies in liquid water and depicted by symbols in Fig. 3. These coefficients follow a linear relation with the proton energy E in a log–log scale, which leads to the expression.

$$C_i = b_i E(\text{MeV})^{a_i}, \quad (5)$$

where a_i and b_i are given in Table 1. This parameterization allows knowing $\langle r^2 \rangle^{1/2}$ for protons in liquid water as a function of the depth easily for any proton initial energy.

Fig. 3. Symbols are the coefficients C_1 and C_2 corresponding to the proposed parabolic fitting of the r_{rms} as a function of depth z , $\langle r^2 \rangle^{1/2} (\mu\text{m}) = C_1 z (\mu\text{m}) + C_2 (\mu\text{m}^{-1}) z^2 (\mu\text{m}^2)$, for protons in liquid water at several projectile initial energies. Solid lines are the fit obtained by Eq. (5), and dashed lines represent their absolute error; in the case of C_2 the dashed lines corresponding to the error are indistinguishable from the solid line.

Table 1

Parameters a_i and b_i appearing in the energy dependence of the coefficients C_1 and C_2 , Eq. (5), used to fit the parabolic behavior of the root mean square radius as a function of the depth, Eq. (4).

i	a_i	b_i
1	-0.058 ± 0.008	$(9.39 \pm 0.14) \times 10^{-3}$
2	1.868 ± 0.010	$(1.56 \pm 0.03) \times 10^{-3}$

4. Summary and conclusions

We have simulated the three-dimensional lateral spread of the deposited dose of proton beams in liquid water by means of the SEICS code, which includes inelastic energy losses, energy-loss straggling, multiple elastic scattering, electron charge-exchange and nuclear fragmentation interactions. We find that the r_{rms} of the particle radial distribution at the Bragg peak depth divided by the Bragg peak depth is independent of the proton energy and has a value around 3%. We also obtain that r_{rms} grows with the depth following a parabola, for all the incident energy range analyzed (5–250 MeV). A parameterization of r_{rms} as a function of the penetration depth and the initial proton energy has been performed, allowing a fast calculation of r_{rms} at any proton energy and depth in liquid water. A comparison of r_{rms} with experimental data and with other analytical models shows good agreement. The multiple elastic scattering results in the lateral spread of the proton dose distribution, being one of the main causes of the spatial degradation of the Bragg peak, with the subsequent loss of precision required for a successful oncological treatment planning. Therefore, a careful characterization of the lateral spread of the dose deposited in biotarget is of importance for improving the accuracy of clinical treatment planning in hadron therapy.

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