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Simulating the radial dose distribution for charged particles in water medium by a semi-empirical model: An analytical approach

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HIGHLIGHTS

- A semi-empirical model based on electronic radiation damage is postulated.
- Analytical approach code and numerical integration were used to deduce the radial dose.
- The radial dose for several heavy ions in liquid water was calculated.
- The proposed model was compared to experimental data.
- The model compared to many Monte Carlo codes (Geant4-DNA) simulation code.

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ABSTRACT

A computational semi-empirical model based on electronic radiation damage to medium has been presented to simulate the radial dose distribution. An analytical approach was used to calculate the deposited energy in water per unit mass within a cylindrical shell of unit length around the ion path at a radial distance between r and $r + dr$, the so-called radial dose distribution, *RDD*. Detail steps were given and the final radial dose integration over the electron range between R_{min} and R_{max} was solved numerically using the *Mid-Point Method*. A validation for the present model was presented by integrating the *RDD* over all possible radial distances, r to yield the tabulated *LET* of the ion. The validation was presented for a range of proton ions of different energies. The *RDD* for heavy charged particles of proton, alpha, Carbon and Oxygen ions of different energies in liquid water were obtained. Good agreement between the present model and experimental, theoretical, and Monte Carlo (Geant4-DNA) data were obtained for all ions under investigations.

1. Introduction

The interaction of charged particle with matter and knowledge of the microscopic distribution of deposited energy around ion tracks, the so-called "radial dose distribution, *RDD*" is the key issue for many applications. In δ-rays theory of track formation the secondary-electrons that produced by the passing ion are the main cause of radiation damage and dose deliver. Delta-ray theory of track formation was first proposed by Katz (Butts and Katz, 1967; Kobetich and Katz, 1968; Katz, 1983) and according to this theory the observed tracks (sometime called end-point) are caused by the interaction of secondary electrons and higher generation electrons with the sensitive element of the detector. The track appearance is ion's charge and energy dependent. Accordingly, *RDD* was assumed as the average energy deposited per unit mass by a charged particle within a concentric cylindrical shell formed between radii r and $r + dr$, where r is the radial distance away from the ion path. Modeling of *RDD* around ion tracks is significant for radiation transport software used for dose simulation in radiobiology at the sub-cellular scale. *RDD* topic is essential for planning the radiation strategy in radiotherapy and is employed to estimate the cell survival rate in the treatment planning system for heavy particle cancer therapy as well (Moribayashi, 2015). It is also used to estimate the single event upset (*SEU*) damage on electronic devices due to heavy ions tracks of high linear energy transfer, *LET* radiations (Boorboor et al., 2015) and finally, assessing and modeling ion-induce damage and modification of materials (Kiefer, 2008; Gupta et al., 2016).

Many simulation codes have been developed for studying radiation transport through matter and calculating the radial dose distribution by the Monte Carlo (MC) method. MC simulation has become an important tool for obtaining detailed information regarding interaction of fast ions

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with matter with the inclusion of all primary excitation and ionization events accompanying the passage of these ions through matter and the microscopic distribution of the deposited energy around ion tracks (Hamm et al., 1985; Emfietzoglou et al., 2004; Wiklund et al., 2009; Bäckström et al., 2013; Nikjoo et al., 2016). Therefore, MC simulation is considered to be one of the most accurate methods for transport of radiation in various media. However, simulating electron scattering in materials in full detail can be time-consuming and impractical for some routine applications (Bousis et al., 2011).

Geant4-DNA (Incerti et al., 2014; Bernal et al., 2015) is one of the high sophisticated MC codes that can be employed for detailed simulation of dose distributions. Comparing the present work to Geant4-DNA toolkit data is essential to raise the confident in the present work. In Geant4-DNA simulation p, α-particles, C and O ions of different energies were shot into liquid water and energy deposition around the particle track were scored in concentric cylindrical shells around the incident particle track. Each shell has a thickness of 1 nm. The MC radial dose profiles for these ions were obtained and compared.

Radial dose distribution was measured experimentally by tissue-equivalent gas where a large ionization chamber consists of an aluminum cylinder and a copper central wire serves as an ion collector. A probe is attached to a long aluminum tube, which can be rotated into various radial positions from the center to almost the wall of the large chamber and a faraday cup was used to determine the beam intensity. The ionization current was measured using a vibrating read electrometer where ionization was converted to energy deposited. The experimental data for 1 MeV proton, 3 MeV alpha (Wingate and Baum, 1976), 24 MeV Carbon (Fain et al., 1974) and 41.1 MeV Oxygen (Varma et al., 1977) were collected and used for comparison with present module calculations. Recently, *RDD* can also be determined experimentally by using solid state thermoluminescent (TL) detectors (Gieszczyk et al., 2014).

Modeling and predicting the radial dose both near and far from the path of the ion is not an easy task because of uncertainties in the electron range-energy relation, the angular dependence of secondary electrons production cross section, and the variation in δ-rays transport theory in matter, especially for condensed-phase matter. Variation and uncertainties in electron-energy loss models is a major obstacle for such code developments (Emfietzogloua and Nikjoo, 2005). Therefore, the original *RDD* formula was constructed using a number of simple assumptions that will be given in the next part. The radial dose distribution, *RDD* from the ion path was first introduced by Butts and Katz in the 1960s (Butts and Katz, 1967; Kobetich and Katz, 1968). This pioneer approach by Katz and co-workers led to formulate biophysical models. This model will be referred to in the present work as "Katz model" for comparison and is given by

$$D(r) = N\frac{Z^{*2}e^4}{\rho m v^2}\frac{1}{\alpha r^2}\left(1-\frac{r}{R}\right)^{\frac{1}{\alpha}} \quad (1)$$

Where R is the range of the ejected electrons in cm and it is given by

$$R = \rho k T^{\alpha} \quad (2)$$

T is the energy of the emitted electrons in keV, $k = 6 \times 10^{-6}$ in (g cm^{-2} keV$^{-\alpha}$), ρ is the density of the target, v is the velocity of impact ions, e and m are the electron charge and mass respectively, N is the number of electrons per unit volume element and, Z^* is the effective charge number of the ion, which is calculated according to Barkas' formula as $Z^* = Z(1-e^{-125\beta Z^{-\frac{2}{3}}})$ and β is ion velocity relative to velocity of light in vacuum. For $T < 1\,keV$ $\alpha = 1.079$ and for $T \geq 1\,keV$ $\alpha = 1.667$.

An improved *RDD* formula was developed (Zhang et al., 1985) where a power law energy-range relationship for electrons was implemented and in 1994 Zhang and co-workers re-calculated the *RDD* sing a logarithmic polynomial to describe the range-energy relationship of electrons (Zhang et al., 1994). It will be referred to in the present work for comparison under "Zhang model" and is given by

$$D(r) = \frac{Ne^4Z^{*2}}{\alpha mc^2\beta^2 r}\frac{\left(1-\frac{(r+\theta)}{(R+\theta)}\right)^{\frac{1}{\alpha}}}{r+k\theta} \quad (3)$$

Where $\theta = kI^{\alpha}$, I is ionization potential of the absorbing medium, k and α as stated for Eqs. (1 and 2).

Waligórski et al. (Waligòrski et al., 1986) developed a semi-empirical analytical formula for *RDD*. They combine the Monte Carlo calculations of the energy deposition due to primary excitations and ionizations of protons in liquid water of different energies into the semi-empirical formula deduced by Zhang (Eq. (3)) and using the electron energy-range (Eq. (2)). They also suggested a corrected *RDD* formula as follows:

$$D_1(r) = D(r)+(1+k(r)) \quad (4)$$

Where *D(r)* is Eq. (3) and *k(r)* is a corrected function that depends on *r*. They were able to reproduce the ion's stopping power of ions of different charges and speeds with high accuracy. The results of this model will be compared to the present work and will be referred as "Waligórski model".

A simple analytical model of ion track structure based on classical collision dynamics were introduced by Kiefer and Straaten (Kiefer and Straaten, 1986). The energy deposition in ion tracks as a function of radial distance, using the simple empirical range-energy relationship of Eq. (2), was used. They were able to deduce a simple formula for *RDD* calculations with reasonable accuracy. The maximum extension of δ-ray in the target (penumbra radius) formula was also deduced.

It is worth noting that these *RDD* models and others had many modifications and improvement during the last few decades and still (Katz, 1978, 1983; Katz et al., 1985; Cucinotta et al., 1995, 1999; Kramer, 1995; Chan and Kellerer, 1997).

It is known that Eq. (2) is a simple energy-range relation of the electron and approximately correct for electron energies above 1000 eV and becomes increasingly incorrect for electron energies below 1000 eV indicating one important limitation of the last models and its potential for improvement (Tombrello, 1994). Therefore, another electron range-energy relation must be used and tested in calculating the *RDD*. The main aim of this study is to develop an analytical formula for fast and efficient estimation for radial dose distribution that can be used as an alternative to Monte Carlo simulation code. An algorithm to calculate the radial dose by using a semi-empirical model based on electronic radiation damage to medium was deduced. *RDD* integration was then calculated by using *Mid-Point Method* rule of integration. Radial dose profile for some heavy charged particles, such as, proton, alpha particles, Carbon and Oxygen passing in liquid water were calculated. The accuracy and validation of the present code was tested by integrating the radial dose to yield the tabulated *LET* values of these ions. The estimated *RDD* was compared to experimental data as well as to the data of Katz, Zhang and Waligórski models and Monte Carlo simulation codes.

2. Calculation methodology

A semi-empirical analytical model based on electronic radiation damage in which secondary-electron collision cascade is the main reason for energy and radial dose distribution produced by charged particle in a given medium is introduced. Despite the fact that this topic is not new and the present model is similar and following the steps suggested by Kiefer and Straaten approach (Kiefer and Straaten, 1986; Spohr, 1990) however, it offers a simple alternative to time consuming Monte Carlo simulations and can be conveniently used in hadron therapy dosimetry.

Due to uncertainties in electron-energy loss models, many assumptions for radial dose estimations had been made in the present work as made in many previous works. These assumptions were the dominant