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Calculation of electron trajectory and energy deposition in no screening region

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ABSTRACT

The probability density function (PDF) of energy for inelastic collision is obtained by solving the integro-differential form of the quantity equation with the Bhabha differential cross section for particles with spin 1/2. Hence, the total PDF in no screening region is determined by folding theory with the following two assumptions: (1) the electron loses energy by collision and radiation and (2) the electron velocity does not change with a thin absorber. Therefore, a set of coupled stochastic differential equations based on the deviation and energy loss PDFs for electron is presented to obtain the electron trajectory inside the target. The energy PDFs for an electron beam with incident energy of 15.7 MeV inside aluminum and copper are calculated. Besides, the dose distributions for an electron beam with incident energies of 20, 10.2, 6, and 0.5 MeV in water are obtained. The results are in excellent agreement with the experimental data reported in the literature.

1. Introduction

Computation of the charged particle trajectory in matter is of particular importance in the study of radiobiological effects of the electrons in a target and dose deposition. The radiobiological effects of emitted electrons have been investigated by many authors [1–4]. The theory of ionization of atoms induced by the impact electron is reviewed by Llovet et al. [5]. Various theoretical models are available for the calculation of total cross section, such as Khare model and models by Kim–Rudd, Variens, and Grizinski and Bousis and coworkers for liquid water [6–10]. The number of the electrons emitted from a target increases in no screening region, where the effect of screening of the atomic potential by the outer electrons on the probability density function (PDF) of the bremsstrahlung can be ignored [11]. In accordance with the radius of the Thomas–Fermi atom for Yukawa potential, the electron energy in no screening region is approximately $< 70\, Z^{-1/3}$, where Z denotes the atomic number of the target [12]. The electron trajectory is originated from the bremsstrahlung emission and inelastic collision with atomic electrons as well as elastic scattering from nuclei. The PDF of energy loss for inelastic collision was calculated by Landau [13] and Vavilov [14]. In multiple scattering, the Moliere series can be considered for investigating the deviation of charged particles [15]. Hence, a relative optical-data model for calculating the inelastic scattering within the first-order Born approximation for electrons and positrons is presented by Fernandez Varea et al. [16]. In the previous work, the motion of proton in various materials was calculated by analytical random sampling from Moliere and Landau PDFs [17]. The energy loss of electrons by radiation is important if the electron energy is larger than a few mega-electron volts [18]. The differential cross section for bremsstrahlung was calculated by Bethe and Heitler [12]. However, the Coulomb correction was added to the bremsstrahlung differential cross section by Koch and Motz [19]. The bremsstrahlung emission and inelastic collision were considered by Mathews to investigate the energy loss distribution of an energetic electron beam with incident energy >15 MeV [20,21]. In the case of ignoring the elastic scattering, the results are in agreement with the experimental data when the electron depth in matter is assumed to be 0.01–0.05 times the radiation length.

Several methods and Monte Carlo computer codes are used for computing radiation transport and track structure in the target [22–24]. The track structure methods are based on the solution of analytical equations describing the transport of projectile in the target. In addition, these methods depend on the numerical solution for sampling the model of the projectile interactions with the target. The one-dimensional (1D) deterministic description of ion transport can be solved by the Boltzmann transport equation [25]. The three-dimensional (3D) Monte Carlo track structure codes are used for simulating the individual interactions of a

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projectile with the atoms and molecules in the target based on the elastic scattering and inelastic collision [26]. Hence, the dose deposition can be calculated by the age diffusion equation [27], whose results are not in good agreement with the experimental data for an electron beam traversing water with incident energy of 5–20 MeV [28]. The Monte Carlo track structure code PENELOPE can be used for electron and photon transport in the target and complex geometries in the energy range of 100–1 GeV [29], where elastic scattering, inelastic scattering, and bremsstrahlung emission are considered. In high-energy physics and nuclear experiments, the Monte Carlo code Geant4 can be considered as a toolkit for simulating the passage of particles through target [30]. On the contrary, MCNP and MCNPX are used for the simulation of neutrons and light ions in the target [31,32]. Thus, the MC4 code is based on different condensed-history transport schemes, where it is modified by Bousis for water in the energy range of 1–10 keV [33]. Other Monte Carlo computer codes are tabulated by Nikjoo et al. [34] for various projectiles, media, and projectile energy ranges.

The aim of this study is to calculate the electron trajectory in a target. The PDF of energy loss for an electron in a thin absorber is derived by folding the Landau and bremsstrahlung PDFs. In this case, a set of coupled stochastic differential equations based on the Moliere and energy loss PDFs is presented in no screening region. Therefore, the dose deposition and the PDF for an electron beam with various incident energies in a certain depth are investigated. The results obtained from this stochastic model are in good agreement with the experimental data.

2. Theory and methods

2.1. Energy loss by collision

The integro-differential form of the continuity equation must be solved to obtain the PDF of energy in each interval. According to the Vavilov approach, the integro-differential equation can be solved using the Laplace transform pairs as follows [35]:

$$f(t,\Delta E)=\frac{1}{2\pi i}\int_{K-i\infty}^{K+i\infty} d\tau\,\exp\left[\tau(\Delta E-\overline{\Delta E})-t\int_0^{Q_m} dQ\frac{d\sigma}{dQ}\left(1-\tau Q-e^{-\tau Q}\right)\right], \tag{1}$$

where K and Q represent an arbitrary real constant and the energy transferred in a single collision, respectively; τ is the Laplace transform for Q; $-\overline{\Delta E}$ and $-\Delta E$ represent the mean and total energy loss for an electron in an absorber with thickness t, respectively; and Q_m is the maximum energy transferred to the atomic electron of a target. The Bhabha differential cross section for the energy transferred to an electron between Q and $Q+dQ$ for a projectile with spin 1/2, mass m, energy T, and charge ze is given by [36]:

$$\frac{d\sigma}{dQ}=2\pi r_0^2 m_e c^2\left(\frac{z}{\beta}\right)^2\frac{1}{Q^2}\left[1-\beta^2\frac{Q}{Q_{max}}+\frac{1}{2}\left(\frac{Q}{T+mc^2}\right)^2\right], \tag{2}$$

where β is the velocity coefficient, which can be obtained from kinetic energy T by the relation $(\gamma-1)m_e c^2$, where $\gamma=1/\sqrt{1-\beta^2}$. By substituting Eq. (2) into Eq. (1), the exponential term in Eq. (1) can be solved as follows:

$$\tau(\Delta E-\overline{\Delta E})-\tau t\xi(1+\beta^2)+\kappa\left[\frac{1}{2(m_e c^2+T)^2}\left(z+e^{-z}-1-\frac{z^2}{2}\right)+1-e^{-z}\right]+(\kappa\beta^2+\tau t\xi)[-Ei(z)+\ln z+\gamma_{EM}], \tag{3}$$

where $\xi=2\pi N_a r_e^2 m_e c^2\rho\left(\frac{Z}{A}\right)\left(\frac{z}{\beta}\right)^2$; κ and z denote $t\xi/Q_{max}$ and τQ_{max}, respectively; and γ_{EM} is the Euler–Mascheroni constant. By defining the variable $p=\kappa z$ in Eq. (3), the PDF $f(t,\Delta E)$ can be written in the following form:

$$f(t,\Delta E)=\frac{e^{\kappa(1+\beta^2\gamma_{EM})}}{2\pi i\xi}\int_{K-i\infty}^{K+i\infty} dp\,\exp\left\{\kappa\beta^2\left[-Ei\left(\frac{p}{\kappa}\right)+\ln p-\ln\kappa\right]+p\left[-Ei\left(\frac{p}{\kappa}\right)+\ln p-\ln\kappa+\frac{\lambda_V}{\kappa}-\kappa e^{-p/\kappa}+\frac{\kappa Q_{max}^2}{2(m_e c^2+T)^2}\left(1+e^{-p/\kappa}-\frac{\kappa}{p}-\frac{p}{\kappa}\right)\right]\right\}, \tag{4}$$

where $\lambda_V=(\Delta E-\overline{\Delta E})/t\xi-(1+\beta^2)+\gamma_{EM}$ is the Vavilov parameter. When $\kappa\to 0$, Eq. (4) reduces to the form:

$$f(t,\Delta E)=\frac{1}{2\pi i\xi}\int_{K-i\infty}^{K+i\infty} dp\,\exp\left\{p\left[\lambda_V+\ln p-\ln\kappa-\frac{Q_{max}^2}{2(m_e c^2+T)^2}\right]\right\}. \tag{5}$$

Therefore, by changing the variable $p=iu$, the Landau PDF can be calculated as follows:

$$f(t,\Delta E)=\frac{1}{\pi t\xi}\int_0^{\infty}\exp(-u\ln u-u\lambda_k)\sin\pi u\,du, \tag{6}$$

where the Landau and Vavilov parameters are related to λ_k as:

$$\lambda_k=\frac{\lambda_L}{\kappa}-\ln\kappa-\frac{Q_{max}^2}{2(m_e c^2+T)^2}=\lambda_L-\frac{Q_{max}^2}{2(m_e c^2+T)^2}=\frac{(\Delta E-\overline{\Delta E})}{t\xi}-(1+\beta^2)+\gamma_{EM}-\frac{Q_{max}^2}{2(m_e c^2+T)^2}-\ln\kappa. \tag{7}$$

As the mass of an electron is smaller than that of an atom, the electron can be deflected significantly in the collision process. Therefore, the Bethe–Bloch formula should be modified when the projectile is an electron. In this case, the maximum allowable energy loss for an electron in an absorber with thickness t is $T/2$, where T is the energy of the electron at $t=0$ [37]. Hence, the mean energy loss for an electron in the interval is given by:

$$\overline{\Delta E}=-\int_0^t dt\frac{dE}{dt}. \tag{8}$$

The energy loss of an electron through a thickness t in a target is calculated by the Bethe–Bloch formula as follows [37]:

$$-\frac{dE}{dt}=\xi t\left[\ln\frac{2m_e c^2\beta^2 Q_{max}}{I^2(1-\beta^2)}-2\beta^2-\delta-2\frac{C}{Z}\right]. \tag{9}$$

The mean excitation potential of the target material (I) and the effective atomic number (Z_{eff}) are listed in Table 1 [38,39]. The values for the density correction δ are given by Sternheimer formula [40], and their constants are reported in the literature [37]. Hence, the parameter C denotes the shell correction. As the nature of the proposed model is stochastic, the experimental data are coupled with the theory by considering $f(\delta)$ instead of $\delta+2C/Z$ in the Bethe–Bloch formula. Therefore, if the electron energy in the interval t is considered as a constant, the mean energy loss becomes:

$$\overline{\Delta E}=\xi t\left[\ln\frac{2m_e c^2\beta^2 Q_{max}}{I^2(1-\beta^2)}-2\beta^2-f(\delta)\right]. \tag{10}$$

Table 1
Values of Z_{eff}, Z_{eff}/A, and I for copper, aluminum, and water.

Material	Z_{eff}/A	Z_{eff}	I (eV)
Water	0.5551	7.46	75
Copper	0.4564	29	322
Aluminum	0.4818	13	166