



Contents lists available at ScienceDirect

## Nuclear Instruments and Methods in Physics Research B

journal homepage: [www.elsevier.com/locate/nimb](http://www.elsevier.com/locate/nimb)

# Stopping power and ranges of electrons, protons and alpha particles in liquid water using the Geant4-DNA package

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## ARTICLE INFO

### Article history:

Available online 26 February 2011

### Keywords:

Monte-Carlo  
Geant4  
Geant4-DNA  
Stopping power  
Ranges

## ABSTRACT

This paper presents stopping power and ranges of electrons, protons, and alpha particles in liquid water, calculated using the latest Geant4-DNA processes implemented in the Geant4 Monte Carlo simulation toolkit. Inelastic cross sections are obtained using the first Born approximation and semi-empirical formulas like Rudd's model for ionisation and the Miller and Green formula for excitation. Elastic collisions and vibrational excitations are considered for tracking electrons until complete thermalisation (0.025 eV). A speed scaling procedure with an effective charge screening term was used to compute alpha particle and heavy ion cross sections. Geant4-DNA simulations were carried out using thin liquid water volumes to determine the linear energy loss ( $dE/dX$ ), while larger volumes were used to obtain the particle range. While results converge for highly energetic particles, differences are observed for low energies when the applied theoretical models begin to diverge from each other. Results show a good agreement between the analytical calculations obtained from the models, the Geant4-DNA Monte Carlo simulation predictions and the data published in the ICRU reports. Geant4-DNA processes apply to the following energy ranges: 0.025 eV–1 MeV for electrons, 100 eV–100 MeV for protons and 1 keV–400 MeV for alpha particles in liquid water, however since experimental data for very low energies is scarce and very difficult to obtain these processes could not be thoroughly validated so they are recommended for energies above 1 eV for electrons, 1 keV for protons and 10 keV for alpha particles. Relativistic, highly charged ions were implemented in our own “house” version of the code and will be available in future releases of Geant4.

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## 1. Introduction

Remaining a cheap but effective way to study track structure and energy deposits in matter, Monte Carlo codes have noticeably evolved over the last 10 years. In this paper we present the recently improved Geant4-DNA package [1–3], an extension to the free open source Geant4 Monte Carlo toolkit [4,5]. The extended processes can generate ionising tracks for microdosimetry applications, and they are partially available for download with the Geant4 toolkit from the official Geant4 webpage. The entire package will be available in future releases, once the required testing procedures are complete (December 2010). The physics processes are dedicated to sub-cellular studies. Specific cross sections were calculated for protons, electrons and alpha particles, taking into consideration all possible interactions such as ionisation, excitation, charge transfer and elastic scattering. Inelastic cross sections were calculated using the first Born approximation. For low

energies, corrections were used for electrons, and semi-empirical models replaced the theoretical calculations for protons and alpha particles in liquid water. Processes are available for protons between 100 eV–100 MeV (recommended above 1 keV), relativistic electrons up to 1 MeV, sub-excitation electrons until complete thermalisation at 0.025 eV (recommended down to 1 eV) and alpha particles between 1 keV–400 MeV (recommended above 10 keV), using the Rudd ionisation model and the Miller and Green model for excitation. Carbon ions and high energy alphas (1 MeV/amu–10 GeV/amu) were implemented in a “house” version for testing and validation.

This work is primarily dedicated to applications in radiobiology. One major parameter characterising radiation in this field is the Linear Energy Transfer (LET). Also referred to as stopping power, it represents the mean amount of energy an incident particle transfers to the target medium per unit path length. Furthermore, most of the energy is deposited through the secondary electrons that are produced by the ion's interactions with the target's molecules. The shape of the radial energy deposition around the ion track will depend on the secondary electrons energies and ranges. It is therefore important to characterise the extended processes for studying the

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estimated LET and particle ranges that can be deduced from the code. Simulations are carried out using the Geant4-DNA package, which estimates the ranges and LET of different particles (alphas, protons and electrons) with different kinetic energies. The obtained results are compared to theoretical calculated values and recommended data, including the ICRU reports.

## 2. The GEANT4-DNA physics

Ionisation and excitation inelastic cross-sections were calculated using the Plane-Wave First Born Approximation (FBA). Detailed by Landau and Lifshitz [6] and Bethe [7,8], it is now widely used to calculate inelastic data, which is a main prerequisite for Monte Carlo transport codes. In our case, because water is considered to be the major component of biological tissue, the cross sections mentioned hereafter are related only to liquid water. We considered 5 ionisation states and 5 excitation states for the water molecule, using the latest dispersion model described by Emfietzoglou et al. [9]. Cross sections described by Dingfelder et al. [10,11] are also available as an alternative data set. In short, the dielectric-response function (DRF) of the target molecule is used to calculate the interaction cross sections for incident particles. According to the FBA, energy and momentum transfers are related to the energy loss function (ELF)  $\text{Im}[-1/\varepsilon(E, q)]$ , where  $\varepsilon$  is the complex DRF characterising the target molecule [6]. A short summary shall be presented here; for calculation details refer to [12–19] and [10,11]. The Born double differential inverse mean-free-path (IMFP) is given in terms of energy loss  $E$  and momentum transfer  $q$  by:

$$\frac{d^2\Sigma(T, E, q)}{dE \cdot dq} = \frac{1}{\pi \cdot \alpha_0 \cdot T \cdot q} \text{Im} \left[ \frac{-1}{\varepsilon(E, q)} \right] \theta[q - q_-(E, \tau)] \theta[q_+(E, \tau) - q] \theta[\tau - E] \quad (1)$$

where  $\alpha_0$  is the Bohr radius,  $\tau$  is the particle kinetic energy,  $T = (m/M)\tau$  is the kinetic energy of an electron travelling with the same velocity of the considered particle,  $m$  is the electron mass,  $M$  is the particle mass,  $\theta$  is the Heaviside step function and  $\varepsilon = \varepsilon_1 + i\varepsilon_2$  represents the complex dielectric-response function of the target material. The momentum transfer limits are given as follows:

$$q_{\pm} = \sqrt{2M}(\sqrt{\tau} \pm \sqrt{\tau - E}) \quad (2)$$

The single differential cross section and the integrated IMFP can be obtained simply by the following expressions:

$$\frac{d\Sigma(T, E)}{dE} = \int \frac{d^2\Sigma(T, E, q)}{dE \cdot dq} \cdot dq \quad (3)$$

$$\Sigma(T) = \int dE \int \frac{d^2\Sigma(T, E, q)}{dE \cdot dq} dq \quad (4)$$

However, the most important task in such calculations is the determination of the ELF, also called the “Bethe surface” of the target. This term characterising the medium was thoroughly studied in the literature and also by D. Emfietzoglou for water in its three different phases. The first step is to fit the experimental points of the DRF in the optical limit range ( $q = 0$ ) into a series of Drude equations and then apply the dispersion model for the positive momentum transfer range ( $q > 0$ ). The only available experiments measuring the ELF of water molecules in the optical limit range were reported by Hayashi et al. [20] and Heller et al. [21].

For low energies, when the incident particle speed approaches the speed of electrons orbiting the target molecule ( $<1$  keV for electrons and  $<300$  keV for protons), the FBA is no longer applicable on its own. In this case, for protons, cross sections were calculated using a combination of semi-empirical models like the Rudd for-

mula for ionisation [22,23] and the Miller and Green formula for excitation [11]. For electron ionisation, the FBA is corrected using the exchange term proposed in ICRU report 37 [24] and a simple coulomb field correction, which accounts for the potential energy gained by the incident electron in the field of the target molecule [25]. The cross section for a given energy  $T$  is then calculated for an increased value  $T' = T + B_j + U_j$  for ionisation, where  $B_j$  and  $U_j$  are the  $j^{\text{th}}$  shell binding energy and the electron average kinetic energy on this shell. For excitation:  $T' = T + 2E_j$ , where  $E_j$  is the  $j^{\text{th}}$  excitation energy. Electron propagation is highly governed by elastic scattering, especially at low energies where this process dominates and a particle goes through a series of scatters without losing energy before an inelastic interaction occurs. Elastic collisions are described by two alternative models; the screened Rutherford and the Champion models [26].

In theory, electrons below 8 eV cannot ionise a water molecule, as this energy is lower than the least bounded shell in the target, so they are called sub-excitation electrons. These electrons can still undergo vibrational and rotational excitations and elastic collisions until complete thermalisation (0.025 eV). Lacking a theory that describes accurately such phenomena, experimental cross sections published by Michaud et al. [27] for ice targets were used after a phase-scaling procedure to account for the liquid phase of the molecules [28]. Electron attachment can also occur between  $\sim 8$ –13 eV. Here we have used the experimental results reported by Melton [29]. For electrons of energy exceeding 10 keV, relativistic assumptions are considered. Longitudinal as well as transverse interactions are taken into consideration. The total ionisation cross section is then given by Bousis et al. [30]:

$$\Sigma_j = \Sigma_j^L + \Sigma_j^T \quad (5)$$

where

$$\Sigma_j^L = \frac{2}{\pi \alpha_0 \beta^2(T) mc^2} \left\{ \int_{E_{\min}}^{E_{\max}} dE \int_{k_{\min}}^{k_{\max}} \text{Im} \left[ -\frac{1}{\varepsilon(E, k)} \right]_j \frac{dk}{k} \right\} \quad (6)$$

and

$$\Sigma_j^T = \frac{1}{\pi \alpha_0 \beta^2(T) mc^2} \left\{ \int_{E_{\min}}^{E_{\max}} dE \left[ \text{Im} \left[ -\frac{1}{\varepsilon(E, 0)} \right]_j \right] \times \left[ \ln \left( \frac{1}{1 - \beta^2(T)} \right) - \beta^2(T) \right] \right\} \quad (7)$$

$mc^2$  is the electron rest energy and  $\beta = \frac{v}{c}$  is the ratio of the incident velocity to the velocity of light. The momentum transfer limits are  $k_{\max, \min} = (ch)^{-1} (\sqrt{T(T + 2mc^2)} \pm \sqrt{(T - E)(T - E + 2mc^2)})$ ,  $E_{\min}$  is equal to the binding energy of each shell, and  $E_{\max} = (T + B_j)/2$ .

In addition to ionisation and excitation, the charge transfer process becomes dominant for low proton energies. It occurs when the incident proton captures an electron and becomes a neutral hydrogen atom by ionising a water molecule. The hydrogen can produce ionisations in the medium and can also undergo a stripping process, losing its orbital electron and returning to its ion state. In this case the electron is ejected in the projectile's direction with the same velocity; in this work excitations by hydrogen atoms have been neglected. Proton charge transfer and stripping processes are studied using semi-empirical formulas [11], and hydrogen atoms were tracked using the Rudd model with a term accounting for the screening effect caused by the projectile bound electron.

For alpha particles and heavier ions such as carbon and oxygen, a speed-scaling procedure was adopted using the proton cross sections, assuming that two particles with the same speed have the same cross section multiplied by an effective charge term. The effective charge and electron transfer for alpha particles were modelled using Dingfelder's approach [31,32]:

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