Nuclear Instruments and Methods in Physics Research B 397 (2017) 45–50

Contents lists available at ScienceDirect

Nuclear Instruments and Methods in Physics Research B

journal homepage: www.elsevier.com/locate/nimb

Geant4-DNA simulation of electron slowing-down spectra in liquid water

S. Incerti [a,b,c,d,*], I. Kyriakou [e], H.N. Tran [a,b]

[a] Division of Nuclear Physics, Ton Duc Thang University, Tan Phong Ward, District 7, Ho Chi Minh City, Viet Nam
[b] Faculty of Applied Sciences, Ton Duc Thang University, Tan Phong Ward, District 7, Ho Chi Minh City, Viet Nam
[c] Univ. Bordeaux, CENBG, UMR 5797, F-33170, Gradignan, France
[d] CNRS, IN2P3, CENBG, UMR 5797, F-33170 Gradignan, France
[e] Medical Physics Laboratory, University of Ioannina Medical School, 45110 Ioannina, Greece

ARTICLE INFO

Article history:
Received 12 July 2016
Received in revised form 19 February 2017
Accepted 20 February 2017

Keywords:
Geant4
Geant4-DNA
Slowing-down
Electron
Photon

ABSTRACT

This work presents the simulation of monoenergetic electron slowing-down spectra in liquid water by the Geant4-DNA extension of the Geant4 Monte Carlo toolkit (release 10.2p01). These spectra are simulated for several incident energies using the most recent Geant4-DNA physics models, and they are compared to literature data. The influence of Auger electron production is discussed. For the first time, a dedicated Geant4-DNA example allowing such simulations is described and is provided to Geant4 users, allowing further verification of Geant4-DNA track structure simulation capabilities.

1. Introduction

The Geant4-DNA extension [1–3] of the general purpose Geant4 Monte Carlo simulation toolkit [4,5] proposes to Geant4 users a set of models allowing the simulation of track structures in liquid water. These models can be used for the simulation of electron elastic and inelastic interactions, including ionization, electronic excitation, vibrational excitation and electron attachment, the latter two being of particular importance for the simulation of water radiolysis [6,7]. The main energy-loss mechanism for sub-keV electrons is electronic excitation and ionization of the target atoms or molecules. It is well-known that the cross sections for such collisions are particularly sensitive to whether the target atoms (or molecules) are in the gas or condensed phase [8]. To account for the liquid-phase of water in Geant4-DNA, the dielectric formalism has been used [9]. The key input in this formalism is the choice of model to describe the dielectric response function of the material. For real materials, and especially for liquids (or amorphous solids), the exact calculation of the dielectric function is impractical. Therefore, semi-empirical descriptions of the dielectric function have been developed, that combine theoretical aspects of electron-gas theory with experimental spectroscopy data [10,11]. This approach has been used in the majority of Monte-Carlo track structure codes [12–17] since it is reasonably accurate with little (or moderate) computational cost. For liquid water, the most used models of the dielectric function are those of Ritchie [18], Dingfelder [19,20], and Emfietzoglou [21–24]. In Geant4-DNA the calculation of ionization and excitation cross sections for electron impact is based on the Emfietzoglou model which offers a better agreement with the experimental data for liquid water [25]. In the last public release of the Geant4 toolkit (release 10.2), an improved implementation of this model has been made yielding a new set of excitation and ionization cross sections [26,27]. This development has permitted a more realistic simulation of W values (the average energy loss per ion pair formed during the complete slowing-down of the incident particle) [26] and dose point kernels [27] compared to the "default" Geant4-DNA model [1].

In a continuous effort to verify the validity of such models, Geant4-DNA includes a set of application examples, so called "extended" Geant4-DNA examples. In the last version of the Geant4 toolkit, thanks to these examples, users have the possibility to simulate several physical quantities widely used to evaluate software performance and accuracy:

* Corresponding author at: Division of Nuclear Physics, Ton Duc Thang University, Ho Chi Minh City, Viet Nam
E-mail addresses: sebastien.incerti@tdt.edu.vn, incerti@cenbg.in2p3.fr (S. Incerti).

http://dx.doi.org/10.1016/j.nimb.2017.02.034
0168-583X/

- track structures (extended example named "dnaphysics") [3],
- range, projected range and penetration ("range") [28],
- dose point kernel for isotropic electron sources ("TestEm12")[1] [27,29],
- W-values ("wvalue") [26],
- S-values in spheres of liquid water ("svalue") [30,31].

Although experimental data in the liquid water phase do not currently exist at low energy and in small size targets, preventing from a full validation of Geant4-DNA models *stricto sensu*, such simulated quantities can be compared to literature data, obtained from other Monte Carlo simulations, from analytical calculations or from experimental data in the gas phase, as described in the above listed references.

In the continuation of this verification effort, this work focuses on the simulation of electron slowing-down spectra in liquid water using Geant4-DNA physics models. Such spectra represent the fluence distribution (differential in energy) of both the primary and all subsequent generations of secondary electrons generated through the full slowing-down process. The reader is invited to consult the work of Tilly et al. [32], which includes a brief historical description of the study of slowing-down spectra. These spectra undoubtedly present an interest for radiobiology simulations, where accuracy in space (nanometre scale) and energy (sub-keV scale) is required. Their simulation is therefore another reliable approach to evaluate the performance of the simulation tool. In the following sections, we first describe the selected simulation conditions and then compare Geant4-DNA simulation results to existing literature data, including the earlier work by Vassiliev [33] who presented the first Geant4-DNA slowing-down spectra. For the first time, a new Geant4-DNA example is provided directly in Geant4 for the simulation of such slowing-down spectra.

2. Materials and methods

2.1. Simulation of slowing-down spectra

Slowing-down spectra presented in this work were simulated using Geant4-DNA physics models available in Geant4 release 10.2p01, under the following conditions:

- monoenergetic electrons or photons were shot randomly from an infinite medium of liquid water; in the case of photons, only the first collision was simulated, following the approach proposed in [33].
- two sets of Geant4-DNA physics models were used for electrons: the first set corresponds to the "default" Geant4-DNA physics models [3] and the second set to the newly added "option4" models by Kyriakou et al., fully described in [26,27]; photon models are obtained in both cases from the "Livermore" EPDL-EADL library [34,35]. These sets are assembled into physics constructors which gather all required particles, processes and models (see Table 1).
- a "tracking cut" can be applied during the simulation in order to stop the transport of electrons below a certain kinetic energy threshold, taken here as 9 eV both for the "default" and the "option4" models. Below this threshold, electrons are stopped and their remaining kinetic energy is locally deposited in the liquid water medium.

[1] The "TestEm12" example belongs to the Geant4 category of "electromagnetic physics" examples and is not specific to Geant4-DNA but can be fully used with Geant4-DNA models.

Table 1
List of Geant4-DNA physics model sets (so called "Geant4-DNA physics constructors") used in this work, available in Geant4 10.2p01.

Set of Geant4-DNA models	Corresponding Geant4-DNA physics constructor	Reference
"default"	G4EmDNAPhysics	[2]
"option4"	G4EmDNAPhysics_option4	[26,27]

- the production of Auger electrons from Oxygen can be activated or not, thanks to the Geant4 universal atomic deexcitation package available in all Geant4 electromagnetic physics categories of models, including Geant4-DNA models [36].
- Geant4-DNA physics processes can be activated/deactivated on request. In the presented simulations, elastic scattering was not taken into account since there is no energy loss in this process.
- simulations can be run in multithreaded mode for faster performance.

In order to compare our results to literature data, the scoring of slowing-down spectra was performed at each interaction step of all electrons following the approach documented in [33]: we recorded for each simulation step the kinetic energy (in eV) of each electron undergoing a Geant4-DNA inelastic process in a log-binned histogram, setting for each record a statistical weight equal to the size of the step (in nm). Each histogram bin was normalized to its energy width (in eV) and the full histogram was normalized to the number of primary electrons. Decades on the spectrum energy axis were sliced into 100 bins. Final results were expressed as slowing-down spectra normalized to the absorbed dose in the liquid water medium (in $cm^{-2}\,eV^{-1}\,Gy^{-1}$), using the following scaling factor f, where y represents histogram bin content (in nm/eV), ρ medium density (in g/cm^3) and E incident energy (in eV) (see eg. formula (3) in [32]):

$$f = y\frac{\rho}{E}\times\frac{10^9}{1.6} \tag{1}$$

2.2. The new "slowing" extended example

The Geant4-DNA application used for these simulations is proposed as a new Geant4-DNA "extended" example. All six conditions previously described for the configuration of the simulations can be fully selected using a macro command file provided with the example, thus minimizing coding efforts and easy usage in multithreaded mode. Slowing-down spectra can be directly drawn using the provided ROOT macro [37]. This example will be made available soon in a Geant4 public release.

3. Results and discussion

3.1. Electron case

Simulations were run for five different incident kinetic energies: 100 eV, 1 keV, 10 keV, 100 keV and 1 MeV. Both Geant4-DNA physics constructors were used ("default" or "option4", see Table 1). Incident statistics was set to reach the same level of accuracy as in [33], that is, in our case, typically 10^6 incident electrons for a given incident energy. In these simulations, Auger electron production and sub-excitation processes (vibrational excitation and electron attachment) were activated or deactivated, in order to evaluate their contribution to slowing-down spectra.

We first compared Geant4-DNA simulations to literature data by Hamm et al. [38], Nikjoo et al. [39] and Tilly et al. [32], including in the simulations the production of Auger electrons from water Oxygen, which was not taken into account in Vassiliev's results