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Limitations (and merits) of PENELOPE as a track-structure code

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Abstract

Purpose: **To outline the limitations of PENELOPE (acronym of PENetration and Energy LOss of Positrons and Electrons) as a track-structure code, and to comment on modifications that enable its fruitful use in certain microdosimetry and nanodosimetry applications.**

Methods: **Attention is paid to the way in which inelastic collisions of electrons are modelled and to the ensuing implications for microdosimetry analysis.**

Results: **Inelastic mean free paths and collision stopping powers calculated with PENELOPE and two well-known optical-data models are compared. An *ad hoc* modification of PENELOPE is summarized where ionization and excitation of liquid water by electron impact is simulated using tables of realistic differential and total cross sections.**

Conclusions: **PENELOPE can be employed advantageously in some track-structure applications provided that the default model for inelastic interactions of electrons is replaced by suitable tables of differential and total cross sections.**

Keywords: Radiation physics, Monte Carlo simulation, microdosimetry

Introduction

Monte Carlo (MC) techniques have become essential tools to describe radiation transport in matter. In microdosimetry applications, liquid water plays a central role as a surrogate for biological media. Hence, a number of track-structure MC codes have been developed over the years to simulate the propagation and interaction of electrons and light ions in this substance (Nikjoo et al. 2006). In principle, general-purpose MC codes may be used as well to simulate electron tracks in liquid water. However, the generic cross sections currently implemented in these programs are unable to reproduce the finest details of the interactions in a condensed medium like water in the liquid state.

PENELOPE (acronym of PENetration and Energy LOss of Positrons and Electrons) (Salvat et al. 2008) is a general-purpose MC code for the coupled transport of electrons, photons and positrons in arbitrary material systems. The databases of cross sections cover the energy interval from 50 eV up to 1 GeV. PENELOPE offers the possibility to track electrons in a 'detailed' (i.e., event-by-event) mode. This feature prompted a number of researchers to employ the program in various microdosimetry studies. Thus, Stewart et al. (2002), Mainardi et al. (2004), Hugtenburg et al. (2007), Hsiao and Stewart (2008), Hugtenburg (2008) and Bernal and Liendo (2009) have pointed out that PENELOPE performs quite well for some microdosimetry problems when operated in an event-by-event mode. However, Bernal and Liendo (2009) and others have reported on the appearance of artifacts in certain simulation results. These shortcomings obviously arise because PENELOPE does not qualify as a track-structure MC code.

In this context, the main purpose of the present article is to highlight the reasons that prevent the successful use of PENELOPE in microdosimetry. In order to circumvent the most serious of these limitations one needs to replace the default model for electron inelastic collisions by a set of cross sections specifically tailored to describe the energy-loss interactions of electrons in liquid water. The work done along these lines by González-Muñoz et al. (2011) is briefly mentioned.

Limitations and merits of PENELOPE as a track-structure code

Most of the models in PENELOPE are accurate enough to describe reasonably well the interactions of electrons in liquid water even at low energies around 100 eV. For instance, the database of cross sections for elastic scattering was computed within the static-exchange approximation using partial-wave methods (International Commission on Radiation Units and Measurements [ICRU] 2007)[1]. This formalism is basically the same as the one underlying the corresponding databases of various microdosimetry codes, e.g., CELLDOSE (acronym of CELL DOSE) (Champion et al. 2008).

On the other hand, the features that limit the capability of PENELOPE (as distributed by the Organisation for Economic Co-operation and Development Nuclear Energy Agency

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[OECD/NEA][2]) to simulate accurately electron tracks in liquid water are the following;

- Cross sections for the various interaction mechanisms pertain to isolated atoms, and mean free paths are rescaled to the actual mass density of the traversed medium. This simplification is implicit in most, if not all, general-purpose MC codes, and is tantamount to the complete neglect of aggregation effects, which are appreciable for low-energy electrons moving in molecular or condensed media.
- Ionization by electron impact is modelled with a simple generalized oscillator strength, and excitations are disregarded.
- The emission of fluorescent radiation (characteristic X-rays and/or Auger electrons) is decoupled from the ionization of atomic inner shells; this simulation strategy may induce negative energy imparted in small scoring volumes.
- The smallest absorption (i.e., cut-off) energies of 50 eV allowed in PENELOPE precludes transport of radiations down to the lowest excitation threshold of the water molecule in the liquid phase, which is around 7 eV. Thus, the simulation of electron track-ends is incomplete.

The second of these items deserves a more detailed explanation owing to its relevance for the topic at hand. To this end, let us consider an electron with linear momentum $\mathbf{p}$ and kinetic energy E that undergoes an inelastic collision with a target atom or molecule. The corresponding quantities after the collision will be denoted as $\mathbf{p}'$ and E'. The plane-wave Born approximation constitutes the conventional framework to describe inelastic interactions of charged particles (Inokuti 1971). For the sake of simplicity, formulas are displayed in a non-relativistic fashion, although the actual implementation in PENELOPE is fully relativistic. Moreover, proportionality factors that are not essential for the present discussion are omitted from the equations altogether; the complete formulas can be found in (Salvat et al. 2008). In the plane-wave Born approximation, the doubly differential cross section may be expressed in terms of the momentum transfer $\mathbf{q} \equiv \mathbf{p} - \mathbf{p}'$ (whose modulus is $q = |\mathbf{q}|$) and the energy transfer $W \equiv E - E'$ as:

$$\frac{\mathrm{d}^2\sigma_i}{\mathrm{d}q\mathrm{d}W} \propto \frac{\mathrm{d}f_i(q,W)}{\mathrm{d}W}, \tag{1}$$

where the generalized oscillator strength of the active shell i, which has N_i electrons and binding energy U_i, is given by:

$$\frac{\mathrm{d}f_i(q,W)}{\mathrm{d}W} \propto \left| \left\langle \psi_f \left| \exp(\mathrm{i}\mathbf{q}\cdot\mathbf{r}/\hbar) \right| \psi \right\rangle \right|^2. \tag{2}$$

In the matrix element, ψ_i and ψ_f are the initial (bound) state and final (bound or free) state of the active electron, respectively. The numerical calculation of $\mathrm{d}f_i(q,W)/\mathrm{d}W$ is straightforward (albeit cumbersome) for an atom but far from trivial if the target is a molecule. In addition, handling of bidimensional tables of generalized oscillator strengths is impractical for MC simulation purposes, e.g., for the random sampling of q and W, even with present-day computing resources. Hence the need for simplifications that nevertheless retain the main advantages of the plane-wave Born formalism. The asymptotic behaviours of the generalized oscillator strength provide useful information to devise a simplified form for $\mathrm{d}f_i(Q,W)/\mathrm{d}W$, where the recoil energy $Q \equiv q^2/2m_\mathrm{e}$ (m_e is the electron mass) has been introduced as a convenient variable. In the case of distant interactions, i.e., those with $Q \ll U_i$,

$$\mathrm{d}f_i(Q,W)/\mathrm{d}W \propto \sigma_{i,\mathrm{ph}}(W), \tag{3}$$

where $\sigma_{i,\mathrm{ph}}$ is the photoelectric cross section (in the dipole approximation). For close collisions, namely those with $Q \gg U_i$, it is:

$$\mathrm{d}f_i(Q,W)/\mathrm{d}W \approx N_i\delta(W-Q). \tag{4}$$

Inspired by the asymptotic behaviours of $\mathrm{d}f_i(Q,W)/\mathrm{d}W$, the Sternheimer-Liljequist model adopted in PENELOPE (Salvat et al. 2008) represents the generalized oscillator strength as a 'δ-oscillator'

$$\mathrm{d}f_i(Q,W)/\mathrm{d}W = f_i[\delta(W-W_i)\Theta(U_i-Q) + \delta(W-Q)\Theta(Q-U_i)], \tag{5}$$

where Θ is the Heaviside step function. The first and second terms in this expression correspond to distant and close interactions, respectively. Notice that the excitation spectrum of distant interactions is collapsed into a single resonance energy W_i and that the $\delta(W-Q)$ factor in the second term appears because in close (binary) collisions the target electrons react as if they were free and at rest ($W = Q$). Besides, all inelastic interactions are treated as ionizations. Furthermore, it is assumed that $f_i = N_i$ and, for an insulator like liquid water, $W_i \approx aU_i$[3]. The parameter a is set imposing that the generalized oscillator strength of the atom at $Q = 0$, $\mathrm{d}f(0,W)/\mathrm{d}W = \Sigma_i \mathrm{d}f_i(0,W)/\mathrm{d}W$, leads to the currently accepted mean excitation energy I (ICRU 1984) through the relation

$$Z \ln I = \sum_i f_i \ln W_i, \tag{6}$$

being $Z = \Sigma_i N_i$ the number of electrons in the target atom or molecule.

As an illustration, Figure 1 shows the generalized oscillator strength of liquid water in the optical limit $Q = 0$ as parameterized by Dingfelder et al. (1998, 2008). The partial contributions of the five molecular orbitals are plotted as well. PENELOPE places the resonance energies W_i of equation (5) at 31.4, 64.0 and 1200 eV with oscillator strengths f_i equal to 6, 2 and 2, respectively (the three outermost molecular orbitals are grouped into a single resonance); these values of W_i are obtained when binding energies of 538, 28.5 and 13.6 eV are employed and $I = 75$ eV (ICRU 1984) is inserted in Equation (6).

The differential cross section for distant interactions, which are the most frequent ones, is:

$$\mathrm{d}\sigma_{i,\mathrm{dist}}/\mathrm{d}W \propto \delta(W-W_i). \tag{7}$$

As a consequence, the kinetic energy of the primary electron after the ionizing collision is assigned the discrete value

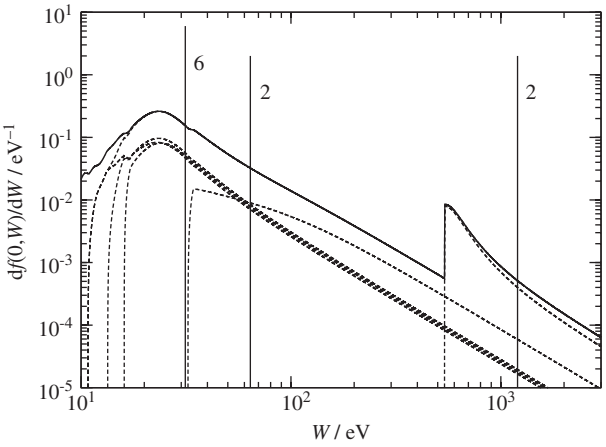

Figure 1. Generalized oscillator strength at $Q = 0$ of liquid water (Dingfelder et al. 1998). The continuous curve is the oscillator strength distribution of one H_2O molecule, encompassing both excitation and ionization, whereas the thin dashed curves are the contributions due to the ionization of the five molecular orbitals. The vertical lines indicate the positions of the resonances W_i, see Equation (5) and the text, and the associated numbers are the corresponding oscillator strengths f_i.

$E' = E - W_i$. The secondary electron gets $E_s = W_i - U_i$ except that the approximation $E_s = W_i$ is made in PENELOPE when U_i is smaller than the absorption (cut-off) energy. These kinetic energies of the outgoing electrons are unrealistic since, as already mentioned, they are not distributed following the actual (continuous) excitation spectrum of the medium. Notice that the energy deposit $E - (E' + E_s) = U_i$ is only correct when $E_s = W_i - U_i$.

The Sternheimer-Liljequist model outlined above yields collision stopping powers of electrons in liquid water which are in good agreement with those tabulated in ICRU Report 37 (ICRU 1984) if the I value recommended in that publication is chosen. This is because the Bethe formula for the collision stopping power, which was used to prepare the tables in that ICRU report, can be derived from the model in the limit $E \gg I$ (Salvat et al. 2008). At lower energies, below a few hundred eV, both the collision stopping powers and the inelastic mean free paths resulting from PENELOPE's algorithm depart from the values calculated with more elaborate approaches such as the optical-data models of Dingfelder et al. (1998, 2008) and Emfietzoglou et al. (2005), which were used to generate the cross section databases included in some track-structure codes. Figure 2 depicts inelastic mean free paths λ and collision stopping powers S computed with these optical-data models and with PENELOPE.

Ad hoc modification of PENELOPE/penEasy

In an attempt to reduce somewhat the aforementioned artifacts caused by the δ-oscillators, Tilly et al. (2002) increased the number of discrete resonances W_i so as to mimic the shape of the $df(0,W)/dW$ distribution. A much better way to remedy for this oversimplification is to replace PENELOPE's algorithm for the simulation of ionizing collisions by a set of tabulated differential and total cross sections pertinent to liquid water, as recently done by González-Muñoz et al. (2011) adapting the structured main program penEasy (Sempau 2008). In particular, the cross sections for the various ionization and excitation channels were computed from [cf. Equation (1)]

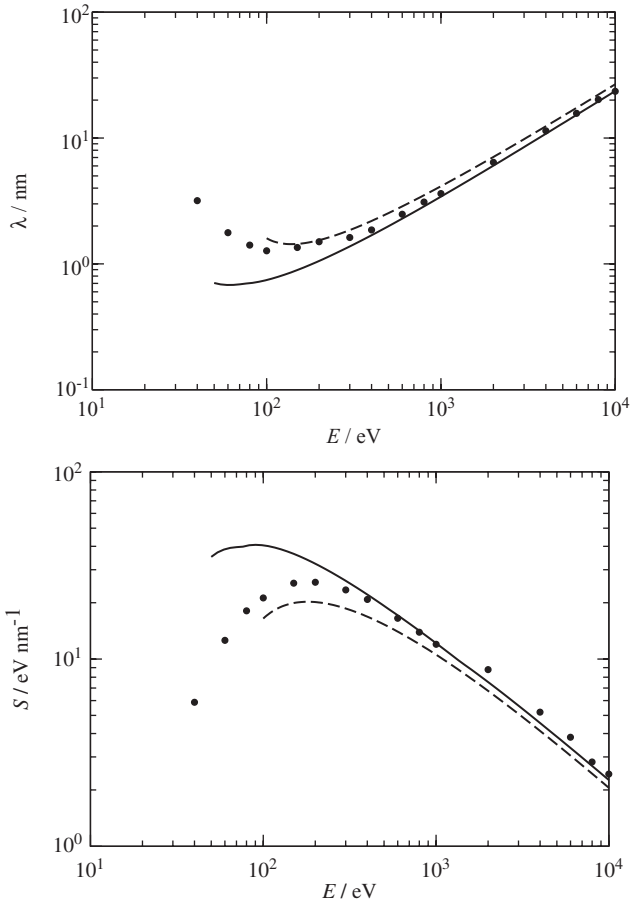

Figure 2. Inelastic mean free path (a) and collision stopping power (b) of electrons in liquid water. The continuous curves are the predictions of the default model in PENELOPE (Salvat et al. 2008), whereas the dashed curves correspond to the fits by Emfietzoglou and Nikjoo (2007) to the results of their optical-data model (Emfietzoglou et al. 2005). The circles are values obtained by Dingfelder et al. (1998).

$$\frac{d^2\sigma_i}{dq\,dW} \propto \frac{\varepsilon_i''(q,W)}{\left|\varepsilon(q,W)\right|^2}, \tag{8}$$

employing Dingfelder et al.'s parameterization of the complex dielectric function $\varepsilon(q,W) = \varepsilon'(q,W) + i\varepsilon''(q,W)$ of liquid water and adding exchange and Coulomb corrections (Dingfelder et al. 1998, 2008). It is worth recalling that these cross sections are incorporated in the PARTRAC (acronym of PARticle TRACk) (Dingfelder et al. 2008) and PITS04 (acronym of Positive Ion Track Structure) (Wilson et al. 2004) track-structure codes. Besides, in order to enforce energy conservation in each energy deposit, either a KLL Auger electron or a Kα characteristic X-ray is released isotropically whenever an ionization occurs in the oxygen K shell.

Incidentally, in the course of a MC investigation on the sensitivity of the spatial extent of electron tracks to the adopted physics models, Wiklund et al. (2011) found that depth-dose distributions of keV electrons simulated using their track-structure code with Dingfelder et al.'s cross sections (Dingfelder et al. 1998, 2008) differ from those generated by PENELOPE even though the two codes rely on the ICRU (2007) database for elastic scattering. PENELOPE's (on average) longer electron tracks came as a surprise because

the selection of $I = 75$ eV for liquid water should yield for $E \gg I$ a larger collision stopping power than that predicted by Dingfelder et al.'s formalism (Dingfelder et al. 1998, 2008) which leads to $I = 81.8$ eV (see Figure 2b). The inconsistency was traced to an anomalous behaviour of their energy-loss function $\mathrm{Im}[-1/\varepsilon(q,W)]$ at intermediate and large values of q, namely that the Bethe sum rule is too high by up to 34%, which may be attributed to the use of truncated Drude functions in ε'' ($q = 0,\ W$) to describe the ionization of the molecular orbitals of H_2O and to the adopted dispersion algorithm. The inelastic mean free path is less sensitive than the collision stopping power to this drawback of the model. Then, the relation $\langle W \rangle = S\lambda$ implies that, on average, energy losses in ionizing collisions will be slightly too large although energy deposits are correctly predicted. In this respect, the analytical representation of $\varepsilon(q,W)$ by Emfietzoglou et al. (2005) might be more consistent because it has recourse to a more realistic dispersion algorithm.

Ongoing work with the modified PENELOPE/penEasy code

A simple MC code, LIonTrack (acronym of Light ION TRACK), has been developed to simulate the slowing down of swift light ions in liquid water (González-Muñoz et al. 2011). The code permits the transport of bare ions H^+, He^{2+}, C^{6+}, etc with specific energies between 0.5 and 300 MeV/u. Ionization differential and total cross sections are precalculated using the continuum distorted wave with eikonal initial state formalism (Galassi et al. 2000). In turn, excitation is described within the first Born approximation resorting to velocity scaling from corresponding electron cross sections as well as scaling with the square of the projectile charge (Dingfelder et al. 2000). Furthermore, LIonTrack assumes rectilinear motion of the ions and disregards nuclear interactions. In this way, the code is suitable for track-segment conditions. LIonTrack generates a 'phase-space file' containing the position, direction and kinetic energy of all electrons ejected by ion-impact ionization along the simulated track segment. These secondary electrons are subsequently transported by the modified PENELOPE/penEasy program down to 50 eV.

The LIonTrack and modified PENELOPE/penEasy codes have been employed to simulate the 3D distribution of energy deposits by ion tracks in liquid water. The clustering capabilities of single ion tracks were then analyzed by looking into the frequencies of distances between energy deposits for several neighbouring orders (1st, 2nd, 3rd, etc nearest neighbours). Other microdosimetry applications include the generation of radial absorbed dose distributions and the calculation of the mean energy imparted by ion tracks in spherical volumes with diameters between 2 and 30 nm (i.e., typical DNA sizes). These simulations and results constitute the subject of a forthcoming publication (González-Muñoz et al. 2011) where they are explained at length.

Conclusions

PENELOPE is a general-purpose MC code whose chief limitation for accurate track-structure applications lies in the manner it simulates inelastic interactions of electrons. The performance of PENELOPE can be improved if the default model is replaced by tables of differential and total ionization and excitation cross sections pertaining to the medium of interest. In particular, cross section tables for liquid water have been linked to PENELOPE/penEasy by González-Muñoz et al. (2011). The modified code permits taking advantage of the rest of PENELOPE's characteristics, such as the coupled electron/photon transport, the flexibility of the geometry package and the possibility of simulation in materials other than liquid water. It can be used in conjunction with a program that stores the initial state of electrons ejected by ion impact, e.g., LIonTrack, to simulate the patterns of energy deposits caused by light ions (González-Muñoz et al. 2011).

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Declaration of interest

The authors report no conflicts of interest. The authors alone are responsible for the content and writing of the paper.

Notes

1. International Commission on Radiation Units and Measurements, URL http://www.icru.org/
2. Organisation for Economic Co-operation and Development Nuclear Energy Agency, URL http://www.oecd-nea.org/
3. The actual relationship between W_i and U_i includes the Lorentz-Lorenz correction (Salvat et al. 2008).

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Note: After completion of this article, a new version of PENELOPE was released where the delta function in eq. (7) is replaced by a continuous (but artificial) distribution.

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