Cross sections for the interactions of 1 eV–100 MeV electrons in liquid water and application to Monte-Carlo simulation of HZE radiation tracks

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Abstract. High charge (Z) and energy (E) (HZE) nuclei are the main contributors to the uncertainty of radiation risk in space. They ionize a large number of molecules when they interact with matter, initiating a complex succession of events that leads to the radiation track structure. Radiation tracks are often studied by Monte-Carlo simulations that provide detailed information on energy deposition and production of radiolytic species that damage cellular components. These simulations require total and differential elastic and inelastic cross sections. Most ionized electrons have low energy; therefore, most calculations and experiments have been performed on electrons below 1 MeV. Electrons of $\sim$1–100 MeV are also produced; they interact with many target molecules when they slow down and determine the radial extension of HZE tracks. Much less work has been done in this energy range. In this paper, a simulation code named RETRACKS uses interaction cross sections (including bremsstrahlung) to calculate the stopping power, range and average energy needed to produce an ion pair ($W$) for electrons up to 100 MeV. It was also used previously with the RITRACKS program to calculate the radial dose of HZE ions. These cross sections should allow the simulation of higher energy HZE ions, which will help improve our models of space radiation risk.
1. Introduction

High charge ($Z$) and energy ($E$) (HZE) nuclei comprising the galactic cosmic rays (GCR) are the main contributors to space radiation risk [1, 2]. The interaction of HZE nuclei with biological matter is often studied by Monte-Carlo track structure simulations that provide detailed information on energy deposition and production of radiolytic species that damage cellular structures [3]. Over 50% of the GCR flux is at energies above 1 GeV amu$^{-1}$ [4]. These nuclei interact with matter and generate a large number of electrons, the majority with energy $<100$ eV [5]. Such electrons are known to produce further ionization and excitations events leading to formation of so-called radiation chemical spurs [6]. At low energy ($<20$ eV), electrons undergo resonant scattering with molecules yielding reactive radicals and molecular species, which can result in DNA breaks and oxidative damage to non-DNA molecules in biological matter [7]. High-energy electrons are also very important in the study of ion track structure because they interact with many more target molecules than low-energy electrons, which generate the so-called penumbra or radial extension of HZE tracks [8]. The extent of the penumbra is determined by the maximum energy of the electrons ionized by the HZE nuclei [9, 10]. The relativistic collision kinematics theory [11] shows that $\sim3.3$ and $\sim136$ MeV electrons can be produced by the interaction of 1 and 10 GeV amu$^{-1}$ $^{56}$Fe with matter, respectively. The range of these electrons in liquid water can be as high as $\sim3$–4 cm; since several high-energy electrons are generated by HZE particles, a single HZE track can affect several cells [12]. Thus, previous estimates of the energy deposition by 1 GeV amu$^{-1}$ $^{56}$Fe
particles have shown that ∼19% of the dose deposited in cells are hit only by δ-rays; for each cell that was traversed by a primary $^{56}$Fe particle, ∼32 cells are hit by δ-rays, each receiving ∼30 mGy (on average) of low-LET radiation [13]. However, irradiated cells may respond by secreting signaling molecules that affect neighboring cells up to 1 mm away [14]; thus, many more cells could be affected by the HZE ion.

In the MeV range, electrons lose their energy mainly by ionization and excitation. Bremsstrahlung collisions contribute ∼0.3% of the energy loss at 1 MeV, and ∼3.7% at 10 MeV [15]; they are neglected in most Monte-Carlo simulation codes of radiation track structure [15]–[19]. However, the contribution of bremsstrahlung to energy loss becomes important above ∼10 MeV. The bremsstrahlung photons are very penetrating and may also contribute to energy deposition far from the core of the track. Since electrons of energies up to 100 MeV are generated by the interaction of HZE particles with matter, energy loss by bremsstrahlung has been included in the simulation program described herein. It is much more difficult to estimate how many cells can be affected by bremsstrahlung photons, since their energy varies from a few keV to a few MeV. Photons interact with matter mainly by the Compton effect, generating Compton electrons and ending their route by a photoelectric effect. Typically, ∼2–15 electrons are generated by photons below 500 keV; ∼15–17 electrons are generated by photons over 500 keV [20]. However, even a 1 keV photon will travel a few microns in water [21]; thus, it can be assumed that the energy deposition events from the bremsstrahlung photon interactions occur in different cells.

Simulations of radiation track structure require total and differential elastic and inelastic cross sections. Unfortunately, measurements of the cross sections for the liquid phase of water are very difficult [5]; thus, simulation codes rely on cross sections obtained by theoretical approaches and semi-empirical models. No existing model is able to fully describe the interaction cross sections of electron with water in the energy range 1–10$^8$ eV. Most calculations and experiments have been performed for electrons of energies below 1 MeV; many fewer have been done over 1 MeV [15]–[19]. The lack of knowledge of the cross sections in this energy range limits the simulation of radiation tracks to ions of energy less than ∼1 GeV amu$^{-1}$. In this work, the ionization, excitation, elastic and bremsstrahlung cross sections from different models are used by a Monte-Carlo electron transport code named RETRACKS to calculate the electron range, stopping power and average energy needed to produce an ion pair ($W$). In general, the calculations are in good agreement with accepted values and results from other simulation codes.

2. Ionization cross sections

Ionization is the most important process for energy loss by electrons >10 eV. Two semi-empirical formulae of the cross sections for the ionization of liquid water molecules by electrons are used in our program. The Rudd model [22] applies to electrons of energy between 1 eV and 50 keV, which represents the overwhelming majority produced by GCR nuclei. Over 50 keV, Seltzer’s equation [15, 16] is used.

2.1. Rudd’s model

The semi-empirical equation of the differential cross section (DCS) of Rudd [22] for electron ionization is adapted from the Mott equation, which takes into account the fact that the
Table 1. Parameters $A_1$, $A_2$, $B_1$ and $B_2$ used in the calculation Rudd’s ionization cross section of the water molecular orbitals.

| Parameter | Liquid  | Inner shells |
|-----------|---------|--------------|
| $A_1$     | 0.94    | 1.31         |
| $A_2$     | 1.13    | 0.37         |
| $B_1$     | 2.30    | 0.00         |
| $B_2$     | 22.0    | 0.00         |

Secondary electrons are indistinguishable from the primaries (Pauli principle).

$$\frac{d\sigma^i_{\text{ion}}}{dW} = \frac{d\sigma^{i(1)}_{\text{ion}}}{dW} + \frac{d\sigma^{i(2)}_{\text{ion}}}{dW}, \quad (1)$$

$$\frac{d\sigma^{i(1)}_{\text{ion}}}{dW} = \frac{S_i}{I_i} F_1(t) \left[ \frac{1}{(1+w)^3} + \frac{1}{(t-w)^3} - \frac{1}{(1+w)^{3/2}(t-w)^{3/2}} \right], \quad (2)$$

$$\frac{d\sigma^{i(2)}_{\text{ion}}}{dW} = \frac{S_i}{I_i} F_2(t) \left[ \frac{1}{(1+w)^2} + \frac{1}{(t-w)^2} - \frac{1}{(1+w)(t-w)} \right]. \quad (3)$$

In equations (1)–(3), the DCS is written as function of the dimensionless quantities $t = T/I_i$ and $w = W/I_i$, where $T$ is the energy of the primary electron, $W$ is the energy of the ejected electrons and $I_i$ is the binding energy of the electron in the $i$th molecular orbital. The multiplicative factor $S_i = 4\pi a_0^2 N_i (\mathcal{R}/I_i)^2$, $a_0$ is the Bohr radius ($5.3 \times 10^{-11} \text{m}$), $\mathcal{R}$ is the Rydberg energy (13.6 eV) and $N_i$ is the number of electrons of the orbital. The functions $F_1(t)$ and $F_2(t)$ are given by

$$F_1(t) = A_1 \frac{\ln(t)}{t + B_1}, \quad (4)$$

$$F_2(t) = \frac{A_2}{t + B_2}. \quad (5)$$

The parameters $A_1$, $A_2$, $B_1$ and $B_2$ (table 1) have been determined by fitting experimental data.

The total ionization cross section (TICS) of the $i$th molecular orbital is found by integrating

$$\sigma^i_{\text{ion}} = \int_0^{E_{\text{max}}+I_i} \frac{d\sigma^i_{\text{ion}}}{dW} dW. \quad (6)$$

The maximal possible energy transfer $E_{\text{max}}$ for both classical and relativistic electrons is $T/2$, because the secondary electrons are indistinguishable from the scattered primaries. This integration gives

$$\sigma^i_{\text{ion}} = S_i F_1(t) \left[ \frac{t - 1}{2t^2} \left( t + 1 - \frac{4\sqrt{t}}{3+t} \right) \right] + S_i F_2(t) \left( 1 - \frac{1}{t} - \frac{\ln(t)}{t+1} \right). \quad (7)$$

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As will be discussed later, this cross section yields excellent results for the calculation of range and stopping power below \( \sim 100 \) keV. Above \( \sim 100 \) keV, the cross section continues to decrease as the energy increases. Our first attempt was to replace \( t \) by a relativistic equivalent
\[
t = \frac{mc^2}{2I} \left[ 1 - \frac{1}{(1 + T/mc^2)^2} \right],
\]
where \( mc^2 = 0.511 \) MeV is the electron rest mass. When \( T \gg mc^2 \), the parenthesis reduces to 1, and \( t \to mc^2/2I_i \), a constant; thus, \( \sigma \) is also constant at high energy. As will be seen later, calculations of stopping power with this cross section gives a plateau at high energy.

2.2. Seltzer's formula

Seltzer's cross section \([15, 16]\) increases over \( \sim 1 \) MeV, which yields a relativistic rise \([23]\) in the calculation of the stopping power. For the \( i \)th orbital of a molecule, the cross-section differential in kinetic energy \( W \) of the ejected electron for an incident electron of kinetic energy \( T \) is written as the sum of two contributions: the close collision and the distant collision:
\[
\frac{d\sigma_i}{dW} = \frac{d\sigma^i_c}{dW} + \frac{d\sigma^i_d}{dW}.
\]
The close collision term is given by
\[
\frac{d\sigma^i_c}{dW} = \frac{2\pi r_e^2 mc^2 N_i}{\beta^2} \frac{T}{T + B_i + U_i} \left[ \frac{1}{E^2} + \frac{1}{(T - W)^2} + \frac{1}{T^2} \left( \frac{\tau}{\tau + 1} \right)^2 - \frac{2\tau + 1}{(\tau + 1)^2} \frac{1}{E(T - W)} + G_i \right],
\]
\[
G_i = \frac{8U_i}{3\pi} \left[ \frac{1}{E^3} + \frac{1}{(T - W)^3} \right] \left[ \tan^{-1} \sqrt{y} + \frac{\sqrt{y(y - 1)}}{(y + 1)^2} \right],
\]
where \( r_e = 2.81794 \times 10^{-15} \) m is the ‘electron radius’, \( mc^2 = 0.511 \) MeV is the electron rest mass, \( \tau = T/mc^2 \) is the kinetic energy in units of the electron rest mass, \( N_i \) is the number of electrons per orbital, \( B_i \) is the binding energy, \( U_i \) is the mean kinetic energy of the target electron in the orbital, \( E = W + B_i \) is the energy transfer and \( y = W/U_i \). The usual relativistic quantities \( \beta \) and \( \gamma \) are:
\[
\beta^2 = \frac{v^2}{c^2} = 1 - \left( 1 + \frac{T}{mc^2} \right)^{-2},
\]
\[
\gamma = (1 - \beta^2)^{-1/2} = 1 + \frac{T}{mc^2}.
\]
The distal collision part of the cross section can be written
\[
\frac{d\sigma^i_d}{dW} = N_i I(E) \sigma_{PE}^i(E).
\]
Here, \( \sigma_{PE}^i(E) \) is the photoelectric cross section for the \( i \)th molecular orbital of water for an incident photon of energy \( E = W + B_i \). They are calculated from the atomic subshell photoelectric cross sections of hydrogen and oxygen by weighting each contribution by the parentage coefficients. These data are taken directly from figure 2 of [15]. The parameters of the molecular orbitals are given in table 2.

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Table 2. Parameters used in the calculation of Seltzer’s equation for the water molecule orbitals $1b_1$, $3a_1$, $1b_2$, $2a_1$ and $1a_1$. $N_i$ is the number of electrons per orbital, $B_i$ is the ionization energy of the orbital, $U_i$ is the mean kinetic energy of the target electron in the orbital and $\langle r_i \rangle$ is the expected value of the radius of the $i$th orbital of the water molecule.

| $i$ | Orbital | $N_i$ | $B_i$ (eV) | $U_i$ (eV) | $\langle r_i \rangle$ |
|-----|---------|------|-----------|-----------|----------------|
| 1   | $1b_1$  | 2    | 11.50 (12.62) | 30        | 0.833          |
| 2   | $3a_1$  | 2    | 11.75 (14.75) | 40        | 0.867          |
| 3   | $1b_2$  | 2    | 13.51 (18.51) | 50        | 0.901          |
| 4   | $2a_1$  | 2    | 16.0 (32.4)   | 60        | 0.906          |
| 5   | $1a_1$  | 2    | 539.7        | 700       | 0.129          |

The quantity $I(E)$ is the virtual-photon spectrum integrated over impact parameters $b_{\text{min}} < b < b_{\text{max}}$.

\[ I(E) = \frac{2}{137\pi\beta^2E} \left[ G(x_{\text{min}}) - H(x_{\text{max}}) \right], \quad (15) \]

\[ G(x_{\text{min}}) = x_{\text{min}}K_0(x_{\text{min}})K_1(x_{\text{min}}) - \frac{x_{\text{min}}^2}{2} \left[ K_1^2(x_{\text{min}}) - K_0^2(x_{\text{min}}) \right], \quad (16) \]

\[ H(x_{\text{max}}) = x_{\text{max}}K_0(x_{\text{max}})K_1(x_{\text{max}}) - \frac{x_{\text{max}}^2}{2} \left[ K_1^2(x_{\text{max}}) - K_0^2(x_{\text{max}}) \right], \quad (17) \]

where

\[ x_{\text{min}} = \frac{Eb_{\text{min}}}{\hbar c} \sqrt{1 - \beta^2}, \quad (18) \]

\[ x_{\text{max}} = \frac{Eb_{\text{max}}}{\hbar c} \sqrt{1 - \beta^2}. \quad (19) \]

Here, $K_0(x)$ and $K_1(x)$ are the modified Bessel function of the second kind [24] of order 0 and 1. The quantities $b_{\text{min}}$ and $b_{\text{max}}$ are impact parameters. That is, $b_{\text{min}} = \langle r \rangle_i$ is the expectation value of the electron radius of the $i$th orbital of the water molecule and

\[ b_{\text{max}} = \frac{1.123\hbar c}{B_i} \frac{\beta}{\sqrt{1 - \beta^2}}. \quad (20) \]

The partial ionization cross section for a molecular orbital is given by

\[ \sigma_i^{\text{ion}} = \int_0^{(T-B_i)/2} \frac{d\sigma_i^{\text{ion}}}{dW} dW. \quad (21) \]

The TICS calculated by summing the cross section for each molecular orbital is shown in figure 1. The transition from Rudd’s to Seltzer’s cross section is at 50 keV. The cross sections for each molecular orbital do not join smoothly at 50 keV, unless the ionization potentials are
Figure 1. Total electron ionization cross section for water calculated by Rudd’s formula for energy <50 keV and by Seltzer’s formula for energy >50 keV. The ionization cross sections of the PARTRAC and NOREC codes [17], from Uehara et al [15] and from Bousis et al [25] are also shown. Experimental data: Djuric et al [26], Schutten et al [27] and Bolorizadeh and Rudd [28].

adjusted. By trial and error, a new set of ionization potentials is found. The most important difference comes from the orbital $2a_1$, for which the ionization potential should be decreased from 32 to 16 eV. To verify our implementation of Seltzer’s equation, the fractional partial ionization cross section has been calculated (not shown). Results similar to figure 4 of [15] have been obtained. The Rudd’s relativistic formula, Seltzer’s cross section (from figure 5 of [15]), calculations from Bousis et al [25], the TICS used in PARTRAC and NOREC codes [17] and experimental data [26]–[28] are also shown. All cross sections are similar. At energies above ~1 MeV, the Rudd’s relativistic formula plateaus, whereas Seltzer’s cross section increases. Bousis et al [25] have performed calculations using both a classical and a relativistic model. The classical model diverges significantly from the other models at high energy.

The ratio of the ionization DCS to the ionization cross section of orbital $1b_1$ for electrons of incident energy of $10^2$, $10^3$, $10^4$, $10^5$ and $10^6$ eV (lines) are shown on figure 2. The DCS of Rudd and Seltzer are very similar. Experimental data [25], [28]–[30] (dots) are also shown. There is a large spread of the DCS experimental data [18]; however, the model used is within experimental uncertainty and is used in similar codes [29, 31].

2.3. Sampling of the energy loss by ionization

To sample the energy loss by ionization, a table lookup method is used:

$$U = \int_0^{w_i} \frac{d\sigma_{ion}}{dW} dW \int_0^{(T-B_i)/2} \frac{d\sigma_{ion}}{dW} dW.$$

(22)
Figure 2. Energy distribution of ionized electrons calculated by Rudd’s formula for $10^2$, $10^3$ and $10^4$ eV incident electrons and by Seltzer’s formula for $10^5$ and $10^6$ eV incident electrons for the molecular orbital $1b_1$ of water. Experimental data: Bolorizadeh and Rudd [28], Vroom and Palmer [30], Kutcher and Green [29] and Bousis et al [25].

The denominator is the total cross section for the ionization shell $i$ and the numerator is the cumulative cross section (the DCS integrated between 0 and $W_s$). A random number $U$ between 0 and 1 is drawn, and the energy $W_s$ corresponding to the random number associated with $U$ is returned. This method is used for sampling the DCS of Rudd and Seltzer.

3. Excitation cross sections

The excitation cross section is lower than the ionization cross section, except at low energies. The relative contributions of each of the electronic excitation levels $\tilde{A}^1B_1$, $\tilde{B}^1A_1$, Ryd A + B, Ryd C + D (Rydberg series), diffuse bands and plasmon excitation (collective excitation) is currently being debated [19, 31]. In our program, only the excitation levels $\tilde{A}^1B_1$, $\tilde{B}^1A_1$ and the plasmon excitation are included [31].

3.1. Excitation cross section of Kutcher and Green [29]

A model of the DCS for losing energy $W$ by excitation of a water molecule has been put forward by Kutcher and Green [29]. It is written as

$$\frac{d\sigma^i_{ex}}{dW} = \rho(W)f_i(W)\ln\left(\frac{4T}{Q_{\text{min}}}\right),$$

(23)

where $T$ is the energy of the incident electron, $\rho(W)$ is the DCS for charged particles on free electrons at rest, $f_i(W)$ are functions that will be defined later and $Q_{\text{min}}$ is the minimum energy
that is transferred in an interaction, given by

\[ Q_{\text{min}} = 2T \left(1 - \frac{1}{2} \frac{W}{T} - \sqrt{1 - \frac{W}{T}}\right). \]  

(24)

The cross section \( \rho(W) \) is

\[ \rho(W) = \frac{e^4}{8\pi\varepsilon_0^2 m^2 v^2} = \frac{4\pi a_0^2}{T} \left(\frac{\mathbb{R}}{W}\right)^2, \]

(25)

where \( a_0 \) is the Bohr radius, \( \varepsilon_0 \) is the vacuum permittivity, \( \mathbb{R} \) is the Rydberg energy, \( m, v \) and \( e \) are the electron mass, velocity and charge. For electrons of energy much higher than the excitation energies, we have \( W/T \ll 1 \). Taylor’s expansion of equation (23) with \( W/T \ll 1 \) yields the result of Magee and Chatterjee [32]:

\[ \frac{d\sigma_{\text{ex}}^i}{dW} = \rho(W) W f_i(W) \ln \left[ \frac{4T}{W} \right]. \]

(26)

This approximation is not valid for electrons of energy close to the excitation energy. For electrons of energy \(<50–100 \text{ eV} \), Kaplan and Sukhonosov [33] have proposed the following equation:

\[ \frac{d\sigma_{\text{ex}}^i}{dW} = \rho(W) W f_i(W) \ln \left[ \frac{T}{W} \right]. \]

(27)

To link the cross section at low- and high-energy, a parameter \( \alpha(T) = 4 - 3\exp[-(W - W_{0,i})/\alpha_i] \) has been introduced in equation (23) by Cobut [34]:

\[ \frac{d\sigma_{\text{ex}}^i}{dW} = \rho(W) W f_i(W) \ln \left[ \frac{\alpha(T)T}{W} \right], \]

(28)

where \( \alpha_i = E_{\text{min}}(\beta^* - 1)/\ln(2) \), \( \beta^* = 5 \) and \( E_{\text{min}} = 7.34 \text{ eV} \) is the minimum energy transfer by excitation [31]. When \( T \to W_{0,i} \), \( \alpha(T) \to 1 \). Similarly, when \( T \to \infty \), \( \alpha(T) \to 4 \). This parameter varies smoothly from 1 to 4. For the excitation of the first level by a 100 eV electron, \( \alpha(T) \sim 3.7 \), which is already close to 4.

The functions \( f_i(W) \) for the excitation levels \( \tilde{A}^1 \tilde{B} \) and \( \tilde{B}^1 \tilde{A}^1 \) are modeled by a Gaussian function [29]

\[ f_i(W) = f_{0,i} \sqrt{\frac{\alpha_i}{\pi}} \exp \left[-\alpha_i(W - W_{0,i})^2\right]. \]

(29)

For plasmons, the function \( f_i(W) \) is

\[ f_i(W) = f_{0,p} \alpha_{pl} \frac{e^\tau}{(1 + e^\tau)^2}, \]

(30)

\[ \tau = \alpha_{pl}(W - W_0). \]

(31)

The parameters \( f_{0,i}, \alpha_i \) and \( W_{0,i} \) are given in table 3.

The excitation cross section is calculated by numerically integrating equation (28):

\[ \sigma_{\text{ex}}^i = \int_{E_{\text{min}}}^{\min(100, T)} \rho(W) W f_i(W) \ln \left[ \frac{\alpha(T)T}{W} \right] dW. \]

(32)
Table 3. Parameters for excitation levels cross sections used in the model of Kutcher and Green [29] for excitation levels $\tilde{A}^1B_1$, $\tilde{B}^1A_1$ and the plasmon excitation.

|       | $\tilde{A}^1B_1$ | $\tilde{B}^1A_1$ | Plasmon |
|-------|-----------------|-----------------|---------|
| $f_{0i}$ | 0.0187          | 0.0157          | 0.7843  |
| $\alpha_i$ | 3 (eV$^{-2}$)  | 1 (eV$^{-2}$)  | 0.6 (eV$^{-1}$) |
| $W_{0i}$ (eV) | 8.4             | 10.1            | 21.3    |

The upper bound is the smallest value between 100 eV and the incident electron energy $T$. These integration limits cover the entire range where the values of the functions $f_i$ are significant, because the $f_i$’s are very narrow peaks between 7.18–9.63 and 7.98–12.2 eV for excitation levels $\tilde{A}^1B_1$ and $\tilde{B}^1A_1$ and between 12.5 and 30.1 eV for plasmon excitation [3].

The classical definition of the kinetic energy $T = \frac{mv^2}{2}$ is used in equation (25) for the calculation of $v^2$. A relativistic version can be obtained by using equation (12) to calculate $v^2$.

### 3.2. Other models of the excitation cross section

Uehara et al [15] have used the empirical formula for the excitation cross section of Berger and Wang [35] in their code:

$$
\sigma_{ex} = 4\pi \left( \frac{a_0}{137\beta} \right)^2 \left\{ 12.30 + 1.26 \left[ \ln \left( \frac{\beta^2}{1 - \beta^2} \right) - \beta^2 \right] \right\},
$$

(33)

where $a_0$ is the Bohr radius and $\beta$ is given by equation (12). The excitation cross sections from the PARTRAC and NOREC codes [17] are also different. The excitation cross sections are compared with our calculations in figure 3. Unfortunately, many fewer data are available for the excitation cross sections; most are obtained indirectly from the energy-loss function of water [36].

### 3.3. Sampling of the energy loss by excitation

The DCS for $\tilde{A}^1B_1$, $\tilde{B}^1A_1$ and plasmon excitation by 1MeV electrons calculated by equation (28) is shown in figure 4. To our knowledge, no experimental data or calculations are available to compare with this model. The energy loss is sampled by a table look-up method like the one described in section 2.3.

### 4. Vibrational and rotational excitations

Experiments on amorphous ice film performed by Michaud et al [37] for 1–100 eV electrons have shown that excitation of vibrational and rotational energy levels of water molecules contributes to the energy loss. In contrast to the excitation states described in the previous section, they do not lead to the dissociation of water molecules.

The cross section for vibrational and rotational excitations has been included in our code. The energy loss is calculated by sampling a Gaussian random number of mean and variance.
Figure 3. Excitation cross sections. Our calculation is the sum of the contribution of the excitation levels $\tilde{A}^{1}B_{1}$, $\tilde{B}^{1}A_{1}$ and the plasmon excitation. The excitation cross section of Berger and Wang [35] and the one used in PARTRAC and NOREC codes [17] are also shown.

Figure 4. DCS of the energy loss of 1 MeV electron by excitation for levels $\tilde{A}^{1}B_{1}$, $\tilde{B}^{1}A_{1}$ and plasmon in liquid water. The area is proportional to the cross section.
Table 4. Excitation energy, full-width at half-maximum (FWHM/2) and anisotropy coefficients for energy loss of low-energy electrons by excitation of vibration and rotation levels [37].

| Mode name | Excitation energy (meV) | FWHM/2 (meV) | Anisotropy coefficient |
|-----------|-------------------------|--------------|------------------------|
| $v'_T$    | 10                      | 0.5          | 0                      |
| $v''_T$   | 24                      | 12.5         | 0.72                   |
| $v'_L$    | 61                      | 15.0         | 0.94                   |
| $v''_L$   | 92                      | 20.0         | 0.99                   |
| $v_2$     | 204                     | 8.0          | 0.96                   |
| $v_{1,3}$ | 417                     | 25.0         | 0.70                   |
| $v_3$     | 460                     | 2.5          | 0                      |
| $v_{1,3} + v_L$ | 500                 | 20.0         | 0.30                   |
| $2(v_{1,3})$ | 835                | 37.5         | 0                      |

given in table 4. For these processes, the electron angular scattering distribution is described by an isotropic component and a forward one of the form

$$\frac{d\sigma}{d\theta} \alpha \cos(\theta).$$

The coefficient of angular anisotropy associated with each excitation mode is used to determine the proportion of each component.

5. Dissociative electron attachment (DEA)

The attachment of an electron to a water molecule leads to the following sequence of events:

$$\text{H}_2\text{O} + e^- \rightarrow \text{H}_2\text{O}^- \rightarrow \text{H}^- + \text{OH}^-.$$

This process is the DEA. In liquid water, H$^-$ will react with a water molecule to produce unscavengeable molecular hydrogen (Jay-Gerin and Ferradini [38]):

$$\text{H}^- + \text{H}_2\text{O} \rightarrow \text{H}_2 + \text{OH}^-.$$

Rowntree et al [39] have given experimental confirmation that DEA occurs in condensed water. It is important only at low energies (~6–7 eV). When it happens, the electron loses all its energy. The DEA cross section has been included in our code.

6. Elastic collisions cross sections

The elastic cross section comes from different models. There is no loss of energy by the electron; thus only the deflection angle should be determined when an elastic collision occurs.

6.1. Electrons of energy below 200 eV

For energies below 200 eV, the experimental elastic cross section of Michaud et al [37] is used. When an elastic scattering event occurs, the semi-empirical DCS parameterized by Brenner and
Zaider [40] is used to sample the angle of deflection. This parameterization is written as

\[
\frac{d\sigma_{el}}{d\Omega} = \alpha(T) \left\{ \frac{1}{1 + 2\gamma(T) - \cos(\theta)} + \frac{\beta(T)}{1 + 2\delta(T) + \cos(\theta)} \right\},
\]

(37)

where \(\alpha(T)\) is a proportionality constant, \(\beta(T), \gamma(T)\) and \(\delta(T)\) are parametric functions in the form of exponentials and polynomials, \(\theta\) is the angle of deflection and \(d\Omega = 2\pi \sin(\theta) d\theta\) is the differential solid angle element in the direction \(\theta\). The total cross section is given by integrating equation (37) over \(d\Omega\):

\[
\sigma_{el} = \frac{\pi}{2} \int_{0}^{2\pi} \frac{d\sigma_{el}}{d\Omega} \sin(\theta) d\theta = \pi \alpha(T) \left[ \frac{1}{\gamma(T)(\gamma(T) + 1)} + \frac{\beta(T)}{\delta(T)(\delta(T) + 1)} \right].
\]

(38)

It is used only to normalize the elastic cross section for testing the sampling algorithms.

6.2. Electrons of energies over 200 eV

Between 200 eV and 150 keV, Cobut et al [31] have used a partial-wave expansion technique to solve the Dirac equation for the spherical double Yukawa potential suited to the water molecule, as proposed by Katase et al [41]. The differential and total cross sections are then calculated from the obtained scattering phaseshifts. We have not been able to reproduce such calculations. The Rutherford cross section with a screening parameter \(\eta\) [15] has been used in our code for energies over 200 eV:

\[
\frac{d\sigma_{el}}{d\Omega} = \frac{Z(Z + 1)r_e^2}{(1 - \cos(\theta) + 2\eta)^2} \frac{1 - \beta^2}{\beta^4}.
\]

(39)

Here, \(r_e\) is the classical electron radius and \(\beta\) is given by equation (12). Equation (39) is relativistic and can be used at high energies. The screening parameter \(\eta\) depends on the atomic number \((Z)\) of the target.

\[
\eta = n_e \frac{1.7 \times 10^{-5} Z^{2/3}}{\tau(\tau + 2)}.
\]

(40)

Integration over \(d\Omega\) yields the total elastic cross section:

\[
\sigma_{el} = \frac{\pi}{2} \int_{0}^{2\pi} \frac{d\sigma_{el}}{d\Omega} \sin(\theta) d\theta = \frac{\pi Z(Z + 1)r_e^2}{\eta(\eta + 1)} \frac{1 - \beta^2}{\beta^4}.
\]

(41)

For a molecular target like water, an effective value \(Z_{eff}\) is used. The values proposed by Uehara et al [15] have been tried to join the experimental results at 200 eV. The value \(Z_{eff} = 7.22\) proposed by Khandelwall [42] has been chosen. The total elastic cross section used in our program is shown in figure 5 and compared with calculations [15, 17, 43] and experimental data [43]–[45]. As for the inelastic cross sections, the elastic cross section yields a plateau at high energy.

6.3. Sampling of the angle of deflection

To generate an angle of deflection for the elastic collision, the DCS is randomly sampled. The DCS of Brenner and Zaider [40] is sampled by a composition method; the DCS of Rutherford is sampled by inversion [46]. Results are shown in figure 6. The experimental results of Trajmar et al [47], Nishimura [48] and Katase et al [41] are also shown.
Figure 5. Elastic cross sections. The cross sections from Michaud et al [37] are used for energies <100 eV. For energies >100 eV, the Rutherford cross section with the screening parameter $\eta$ (see text) is used. The elastic cross sections used by Dingfelder et al [17], Uehara et al [15] and Pimblott et al [43] are also shown. Experimental data: NIST Database [44], Katase et al [41] and Danjo et al [45].

7. Bremsstrahlung

Bremsstrahlung is the most important energy loss process for high-energy electrons. Briefly, the mechanism is energy loss by electromagnetic radiation produced by the deceleration of a charged particle, such as an electron when deflected by another charged particle such as an atomic nucleus or electron. Bremsstrahlung has been extensively studied [49, 50], but it has been included only recently in Monte-Carlo simulation codes such as PENELOPE or EGSnrc [51]. In this work, only the electron–nucleus and electron–electron bremsstrahlung are considered. The bremsstrahlung DCS is often written as

$$\frac{d\sigma_{\text{brem}}(T, Z)}{dW} = \frac{Z^2}{\beta^2 W} \chi(Z, T, \kappa).$$  \hspace{1cm} (42)

Here, $Z$ is the charge of the target, $\beta$ is the velocity of the electron in units of the speed of light $c$ (equation (12)), $\kappa = W/T$ is the energy of the photon ($W$) divided by the incident electron energy ($T$) and $\chi(Z, T, \kappa)$ is known as the scaled energy-loss DCS. The latter is finite for all $\kappa$ and varies smoothly with both $T$ and $\kappa$. A semi-empirical formula for $\chi(Z, T, \kappa)$ exists; however, for this work, the values taken directly from the table of Seltzer and Berger [52] have been used. This table constitutes the most reliable theoretical representation of bremsstrahlung energy spectra available at present [51]. Equation (42) applies for an element $Z$. The bremsstrahlung DCS of a molecule is the sum of the DCSs from its atoms. Consider a molecule $X_xY_y$, comprising $x$ atoms of the element $X$ and $y$ atoms of the element $Y$. The
Figure 6. Elastic DCS. For energies <200 eV, the parametric formulation of Brenner and Zaider [40] is used. For energies >200 eV, the Rutherford cross section is used. The lines are the analytical predictions; the small dots are obtained by sampling the DCS. Experimental data from Trajmar et al [47], Nishimura [48] and Katase et al [41] are also shown.

A quantity $\chi_{\text{mol}}(T, W)$ can be defined as

$$\chi_{\text{mol}}(T, W) = \frac{\beta^2}{Z_{\text{eq}}^2} W \frac{d\sigma_{\text{brem}}(T)}{dW} = \frac{Z_X}{Z_{\text{eq}}^2} \chi(Z_X, T, W) + \frac{Z_Y}{Z_{\text{eq}}^2} \chi(Z_Y, T, W).$$

(44)

with

$$Z_{\text{eq}}^2 = \frac{1}{x+y} (x Z_X^2 + y Z_Y^2).$$

(45)

For water, $Z_{\text{eq}} = 4.69$. The oxygen and hydrogen atoms contribute 80 and 20% of the value of $\chi_{\text{mol}}$, respectively. The bremsstrahlung scaled energy-loss DCS for electrons in water are shown in figure 7 for $10^3, 10^4, 10^5, 10^6, 10^7$ and $10^8$ eV.

In figure 8, the bremsstrahlung DCS is shown for the same incident electron energies. The energy loss is also sampled by using a table lookup method (section 2.3). Figures 7 and 8 show that an electron may lose any fraction of its energy by bremsstrahlung.

The bremsstrahlung cross section is calculated by integrating numerically equation (42):

$$\sigma_{\text{brem}}(T) = \int_0^T \frac{d\sigma_{\text{brem}}(T)}{dW} dW.$$  

(46)
Figure 7. Bremsstrahlung $\chi$ values calculated for water molecules from the tables of Seltzer and Berger [52] for $10^3, 10^4, 10^5, 10^6, 10^7$ and $10^8$ eV electrons.

Figure 8. Bremsstrahlung DCS ($d\sigma/dW$) (lines) for $10^3, 10^4, 10^5, 10^6, 10^7$ and $10^8$ eV electrons calculated from the $\chi$ values shown in figure 7.

The lower bound of integration is a small quantity $0^+$ to avoid the divergence at $W = 0$. Finally, all cross sections are shown on the same graph on figure 9, covering the energy range extending from 1 eV to 100 MeV. The bremsstrahlung cross section is several orders of magnitude lower.
Figure 9. Total ionization, excitation, vibration-rotation, dissociative attachment, elastic and bremsstrahlung cross sections as a function of the electron energy used in RETRACKS.

than ionization or excitation cross sections, even at high energy. The bremsstrahlung cross section is even higher at low energy. This is rather surprising, but similar to data for $^{13}$Al and $^{97}$Au [51]. The effect of bremsstrahlung is seen on the calculation of stopping power, which will be discussed in the following section.

8. Results and discussion

Monte-Carlo simulations of electron tracks have been performed with the new C++ program named RETRACKS. The transport algorithm, which comprises several aspects such as the angular deflection of the incident and ejected electron after ionization and the delocalization of the energy loss, is described in [31]. Early events such as the recombination of an electron with its parent cation, the dissociation of ionized and excited water molecules, plasmon decay and electron thermalization, which leads to the production of the radiolytic species (e_{aq}^{-}, •OH, H•, H₂, H₂O₂, ...), are also described in [31]. Several quantities have been calculated by RETRACKS: the stopping power, the electron range and the $W$ value, which is the average energy needed to produce an ion pair. The code has also been used to calculate the radial dose of HZE tracks [3].

The $W$ value has been calculated with the codes PARTRAC and NOREC by Dingfelder et al [17] by dividing the given incident electron energy by the number of particles produced during the slowing down of the primary and all secondary electrons. They found that the $W$

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3 The RETRACKS program is different from the TRACELE program [27], although many of its features are similar.
value converges to an asymptotical value of 25.4 eV at high energy. The calculation of $W$ has also been done previously with the Notre-Dame code [53], the cpat code [54] and also by Kutcher and Green [29]. Experimental data from Combecher [55] in the gas phase is also shown; their values are significantly higher than most calculations. The $W$ value has been calculated with RETRACKS and we have found the same trend as a function of the energy, with an asymptotic value of $\sim 22.8$ eV (figure 10). Several factors can explain this difference. In our code, an ionized electron has an energy-dependent probability of recombination with the parent cation [56]. The water molecule in the $\tilde{B}^1A_1$ excitation state or the excited plasmon can also lead to ionization [57]. The branching ratios (probabilities) for the dissociation pathway of the excited water molecules have been revised recently by Meesungnoen and Jay-Gerin [57]. From previous papers, it is not possible to know if autoionization of excited water molecules and recombination events have been included in the PARTRAC and NOREC codes. This could change the number of ionizations and thus, the $W$ values.

The range of electrons of energies up to 150 keV has been calculated by Meesungnoen et al [9] and up to 100 keV by Uehara and Nikjoo [58]. Figure 11 displays the computed values of the electron penetration range in liquid water as a function of initial electron energy from 0.1 eV to 10 MeV by using the relativistic and the non-relativistic cross sections. Experimental results from Konovalev et al [59] are also shown. The results obtained below 150 keV are similar to those from Meesungnoen et al [9]; the reader is thus referred to this paper for a more detailed discussion of this curve below 150 keV. Only major points will be recalled here. In the subexcitation electron energy range ($< 7.3$ eV), the penetration range is often called the ‘thermalization distance’. It increases from $\sim 0.35$ nm at 0.1 eV to $\sim 18$ nm at 7.3 eV. This problem has been extensively studied [56]; our values are in good agreement with the

**Figure 10.** Average energy to produce an ion pair ($W$). Calculations from codes PARTRAC and NOREC [17], Notre-Dame [53], cpat [54] and Kutcher and Green [29] are also shown. Experimental data: Combecher [55].
Figure 11. Electron range in liquid water. The calculations have been performed using the classical and relativistic cross sections. Data from Meesungnoen et al [9], Uehara and Nikjoo [58], Watt [61], the CRC Handbook [62] and Konovalov et al [59] are also shown.

reported values. Three minima in the electron range curve are reported [9] at ∼11, 22 and 30–35 eV; however, they are not clearly seen in our calculation shown in figure 11. Between 30 and 300 eV, the calculated range increases very slowly, also in agreement with [9]. To our knowledge, there are no experimental data between ∼5 and 50 eV, where the minima are predicted by Meesungnoen et al [9] and by Uehara and Nikjoo [58]. Between 300 eV and 150 keV, there is an excellent agreement of our calculations with the values from the CRC Handbook [60] and the book by Watt [61]. Over ∼150 keV, the difference in the electron range calculated with the relativistic and the non-relativistic cross sections appears. The relativistic cross sections need to be used for the calculation of the electron range to be in agreement with data from [60, 61]. Many fewer calculations of the electron range have been performed over 1 MeV, probably because these codes did not include the cross sections over 1 MeV.

The stopping power is another very important quantity that we have used to validate our simulation code. The calculation has been performed by Gümüş [23] and Paretzke (see [17]). Stopping power data are found in the CRC Handbook [60], Watt [61], ICRU 37 [62], ICRU 16 [63] and IAEA [64]. The available data for stopping power exist with and without the bremsstrahlung contribution. The stopping power has been calculated by RETRACKS (figure 12) with Rudd’s and Seltzer’s formulae, with and without bremsstrahlung. There is excellent agreement of our code with the existing data in the whole range, but the agreement is best between ∼1 keV and ∼100 keV. In the MeV region, the calculation has been performed by using Rudd’s formula with relativistic corrections and with Seltzer’s formula. The difference is clearly seen in the MeV region. The bremsstrahlung cross section is higher at low energy,
but it is several orders of magnitude smaller than the ionization cross section. This means that bremsstrahlung is a relatively rare event. The DCS explains why it plays a role only at high energy. For all electron energies, the ionization DCS is a plateau up to \( \sim 1–10 \text{ eV} \) and then drops rapidly as \( \sim 1/W^2 \), whereas the bremsstrahlung DCS drops as \( \sim 1/W \). At high incident electron energy, most ionization events are in the low-energy range (\(< 10–50 \text{ eV}\)), but large energy loss events by bremsstrahlung are more likely to occur. Because the electron can lose a significant fraction of its energy during a single bremsstrahlung event, a large dispersion of the points in the stopping power is observed in the MeV region; however, the stopping power clearly increases at high energy and agrees well with [60]. Some Monte-Carlo codes use variance reduction techniques to avoid dispersion of points [51], but we have not used them.

The RETRACKS program has been used along with the HZE track simulation program RITRACKS [3], which generate electrons in the relativistic range. Figure 6 from [3] displays XY plane projections of track segments calculated at \( \sim 10^{-12} \text{ s} \) for \(^4\text{He}^{2+}, ^{12}\text{C}^{6+}, ^{28}\text{Si}^{14+}\) and \(^{56}\text{Fe}^{26+}\) ions (LET \( \sim 150 \text{ keV} \mu\text{m}^{-1}\)). In figure 7 ([3]), the radial distribution profile of the primary radiolytic species (H\(^•\), •OH, H\(_2\), H\(_2\)O\(_2\), and e\(_{aq}^-\)) at \( \sim 10^{-12} \text{ s} \) of these tracks is shown. In figure 8 ([3]), the calculated radial dose is shown for \(^1\text{H}^+\) (1 MeV amu\(^{-1}\), LET \( \sim 33 \text{ keV} \mu\text{m}^{-1}\)), \(^{20}\text{Ne}^{10+}\) (377 MeV amu\(^{-1}\), LET \( \sim 31 \text{ keV} \mu\text{m}^{-1}\)), \(^4\text{He}^{2+}\) (0.55 MeV amu\(^{-1}\)) and \(^{56}\text{Fe}^{26+}\) (1 GeV amu\(^{-1}\)) (LET \( \sim 150 \text{ keV} \mu\text{m}^{-1}\) for both ions). The calculation of the radial dose uses the electron track structure code described in this paper. The good agreement with existing
experimental data provides a validation of this program. These figures also illustrate the fact that the extent of the penumbra increases with increasing charge and energy per nucleon for the same LET value, because the maximum energy transferred from the ion to an electron in an ionization increases with the energy per nucleon.

The increasing interest of NASA for a 3-year Mars mission raises concerns for the health risks associated with GCRs, which are made up of HZE particles. Such radiation produces electrons of a wide range of energy, including delta-rays that can have energies that extend well into the relativistic energy ranges. These electrons interact with many target molecules and are important in determining the extent and range of the penumbra for these ions [12, 65]. On the other hand, electrons with energies below a few keV [7] are known to damage DNA and other biomolecules with higher efficiency than higher energy electrons. It is thus very important to describe accurately the electron tracks to assess the risk of these ionizing radiations. As cross section data for liquid water are scarce, most simulation codes rely on analytical and semi-empirical models. This work has shown that data consistent with other calculations and experiments can be obtained by using the present models in the calculation of important dosimetric quantities like the electron energy range, stopping power, W values and radial dose distribution for HZE particles. Furthermore, we have shown that high-energy electrons generated by the interaction of HZE particles with matter can lead to energy deposition very far from the original track structure, because of their long range (>3–4 cm) in liquid water and bremsstrahlung collisions which lead to the creation of photons. Thus, several cells may be affected by a single HZE ion. These simulation studies should be valuable to improve our models to assess the biological risk associated with HZE nuclei comprising the GCR to which astronauts are exposed during prolonged space exploration missions or in cancer therapy with heavy ions.

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