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Collision of Incident Electrons with Liquid Water Molecules: Study of Linear Energy Transfer (LET)

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Authors' contributions

This work was carried out in collaboration among all authors. All authors read and approved the final manuscript.

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ABSTRACT

We used GAMOS software to simulate the interaction of electrons in liquid water. In our work, the chosen parameter, the Linear Energy Transfer (LET), is studied in an energy range from 2.5 eV to 100 MeV. The results obtained were analyzed and compared with experimental data and literature. A very good agreement emerged.
Also the analysis of the LET curve of the medium crossed presents a maximum of 37.0626 MeV/mm corresponding to an electron energy of 102.447 eV. For energies below this value, the energy loss is greater. On the other hand, for energies higher than this value, there is less energy loss.

Keywords: Electron; liquid water; ionization; collision; GAMOS; GEANT4; LET.

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1. INTRODUCTION

Many scientific researches are often expensive or the conditions of their realizations remain inaccessible. They are however necessary to improve our knowledge and achieve progress. However, to overcome these limitations or difficulties (obstacles), simulations could be carried out [1,2]. This is how the second half of the 20th century saw the development of modeling and simulation tools. The Monte Carlo method has seen increasing use, aided by the growing availability of computers and other means of calculation. Nowadays these simulations find a lot of application in various fields of research and development [3-5].

In particular, many Monte Carlo codes are dedicated specifically to the transport and study of particle interactions. Simulation makes it possible to save time and to study accidental situations or uses in hostile mode inaccessible to experience [6,7]. This is why we use the Monte Carlo simulation software based on the Geant4 toolbox [8,9], with the acronym GAMOS which stands for “Geant4-based Architecture for Medicine-Oriented Simulations”. This software has the advantage of being in free access (Open Access) to simulate the interactions of electrons in liquid water and offers a certain user-friendliness [10].

In the present article, we chose to study the interactions of electrons with water molecules considering the importance and abundance of water in the biological cell in order to better elucidate the consequences. This study was conducted using the GAMOS software which made it possible to carry out the simulations. The results obtained will be presented and discussed.

2. MATERIALS AND METHODS

2.1 Materials

A GAMOS platform [10], based on the Geant4 Monte Carlo technique [8], was used to simulate the impact of electrons with liquid water molecules.

As part of our work, we simulated, with the GAMOS software, the water molecules (“G4_WATER”, density 1.0 gcm-3) contained in a rectangular parallelepiped of dimension 4*cm 4*cm*0.5cm; We also simulated the primary electron beam of 100 MeV located in a 10 degree cone and at -10cm from the position of the water molecules along the z axis. The whole is placed in a volume called “world” represented by a box of dimension 10*cm 10*cm 20*cm filled with air (see Fig. 1).

2.1.1 Physics

The ionization is modeled by the Moller-Bhabha formulation [Physics Reference Manual Release 10.5, 2019].

The GEANT4 collaboration [11] defines a process as a C++ class that describes how and when a type of physical interaction occurs along a particle's trajectory. A wide range of physical processes can be simulated with GEANT4. These processes are grouped into seven (7) categories: electromagnetic, hadronic, decay, optical, photolepton-hadron, parameterization and transportation. In this simulation the electromagnetic processes and the transport process have been taken into account.

In our simulation, we adopted the parameterizations of the electromagnetic interactions optimized (GmEMExtendedPhysics physics package), in which all the electromagnetic processes for incoming photons (Rayleigh and Compton scattering, photoelectric effect, pair production) and charged particles (elastic and multiple scattering, ionization, bremsstrahlung emission, annihilation) are taken into account, as described in the GAMOS user guide and in the GEANT4 Physics reference manual [Physics Reference Manual Release 10.5, 2019]

These GEANT4 processes inherit from the G4VProcess class and are implemented generically. Each process must be able to simulate at least one of these actions: continuous (AlongStep), discrete (PostStep) or stopped (AtRest). For each action, the GetPhysicalInteractionLength (GPIL) method determines where the interaction takes place and the DoIt method generates the final state of the particle. The G4eIonization class provides the calculation of continuous or discrete energy loss due to ionization in a material [Physics Reference Manual Release 10.5, 2019].

2.2 Methods

Considering ionization as the dominant process that contributes to electron energy loss for energies above 10 eV. For this purpose, two

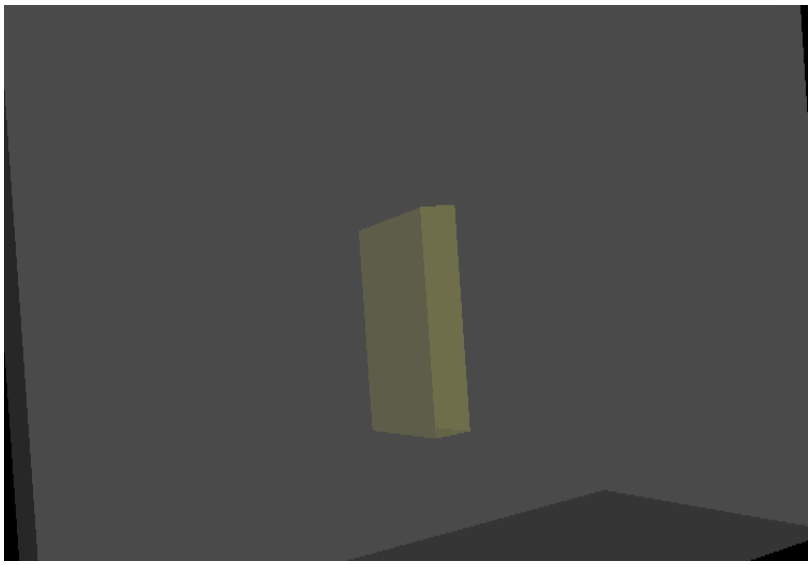


Fig. 1. Geometry without electron beam in GAMOS

semi-empirical formulas of the cross sections for the ionization of liquid water molecules by electron impact are used. These are the Rudd model [12] for electrons with energies between 1 eV and 50 keV and the Seltzer equation for energies above 50 keV [13,14]. Ionization leads to the loss of continuous and discrete energy in a material. Below a given energy threshold, the energy loss is continuous and above it, the energy loss is accompanied by secondary particles.

In our work, the chosen parameter is represented over an energy range extending from 2.5 eV to 100 MeV.

3. RESULTS AND DISCUSSION

Monte-Carlo simulations of electron traces have been carried out. The transport algorithm, which includes several aspects such as the angular deviation of the incident and ejected electron after ionization and the delocalization of the energy loss, is described in Cobut [15]. The simulation on GAMOS allowed us to determine the Linear Energy Transfer (LET).

The GAMOS software is based on the Geant4 toolkit [8,9].

Any energy loss process in GEANT4 must calculate the continuous and discrete energy loss in a material. Below a given energy threshold, the energy loss is continuous and above this, the energy loss is simulated by the explicit production of secondary particles such us electrons.

Either $$\frac{d\sigma(Z,E,T)}{dT} \quad (1)$$

the differential cross section per atom (atomic number Z) for the ejection of a secondary particle with kinetic energy T by an incident particle of total energy E moving in a material of density ρ. The value of the cut-off or kinetic energy production threshold is denoted T_{cut}. Below this threshold, the ejected secondary electrons are simulated as continuous energy loss of the incident particle and, above it, it is explicitly generated. The average energy rate is defined by:

$$\frac{dE_{soft}(E,T_{cut})}{dx} = n_{at}.\int_0^{T_{cut}} \frac{d\sigma(Z,E,T)}{dT} TdT \quad (2)$$

where n_{at} is the number of atoms per volume in the material. and T_{max} is the maximum energy transferable to the secondary particle.

The G4eIonisation class provides the continuous and discrete energy losses of electrons due to ionisation in a material according to the approach described in Mean Energy Loss. The value of the maximum energy transferable to a free electron $T_{\max}$ is given by the following relation:

$$T_{\max} = \frac{\left(E - mc^2\right)}{2} \quad (3)$$

where mc^2 is the electron mass

Above a given threshold energy, the energy loss is simulated by the explicit production of delta rays by Möller scattering, or Bhabha scattering. Below the threshold the soft electrons ejected are simulated as continuous energy loss by the incident electron.

By integrating the relation (2), we obtain:

$$\left.\frac{d\ddot{E}}{dx}\right]_{T<T_{cut}} = 2\pi r_e^2 mc^{\acute{e}} n_{el} \frac{1}{\beta^2}\left[\ln\frac{2(\gamma+1)}{\left(\frac{I}{mc^{\acute{e}}}\right)^2} + F^{\pm}(\tau,\tau_{up}) - \delta\right] \quad (4)$$

Where :

$$r_e = \frac{e^2}{4\pi\varepsilon_0 mc^2} : classical\ electron\ radius$$

$$mc^2 : \text{mass energy of the } electron$$

$$n_{el} : electron\ density\ in\ the\ Liquid\ water$$

$$I : mean\ excitation\ energy\ in\ the\ Liquid\ water$$

$$\gamma = \frac{E}{mc^2}$$

$$\beta^2 = 1 - \frac{1}{\gamma^2}$$

$$\tau = \gamma - 1$$

$$T_{cut} : minimum\ energy\ cut \text{ for } \delta\text{-}ray\ production$$

$$\tau_c = \frac{T_{cut}}{mc^2}$$

$$\tau_{\max} : maximum\ energy\ transfer = \frac{\tau}{2}\ for\ the\ electron$$

$$\tau_{up} = \min\left(\tau_c, \tau_{\max}\right)$$

$$\delta : density\ effect\ function.$$

The functions $F^{\pm}$ are given by:

$$F^{+}(\tau,\tau_{up}) = \ln(\tau\tau_{up}) - \frac{\tau_{up}^2}{\tau}\left[\tau + 2\tau_{up} - \frac{3\tau_{up}^2 y}{2} - \left(\tau_{up} - \frac{\tau_{up}^3}{3}\right)y^2 - \left(\frac{\tau_{up}^2}{2} - \tau\frac{\tau_{up}^3}{3} + \frac{\tau_{up}^4}{4}\right)y^3\right] \quad (5)$$

$$F^{-}(\tau,\tau_{up}) = -1 - \beta^2 + \ln\left[(\tau - \tau_{up})\tau_{up}\right] + \frac{\tau}{\tau - \tau_{up}} + \frac{1}{\gamma^2}\left[\frac{\tau_{up}^2}{2} + (2\tau+1)\ln\left(1 - \frac{\tau_{up}}{\tau}\right)\right] \quad (6)$$

Where

$$y = \frac{1}{\gamma + 1}$$

These values are pre-calculated during the initialization phase of GEANT4 and stored in the table $\frac{dE}{dx}$.Using this table, particle ranges in given materials are calculated and stored in the Range table. The Range table is then inverted to provide the InverseRange table. At runtime, the values of continuous energy loss and particle range are obtained using these tables.

We simulated, with the GAMOS software, through a script, the water molecules ("G4_WATER", density 1.0 gcm-3) contained in a rectangular parallelepiped of dimension 4*cm 4*cm*0.5cm; (see Fig. 1).

The whole is placed in a volume called "world" represented by a box of dimension 10*cm 10*cm 20*cm filled with air (see Fig. 1).

Fig. 1 shows the image of the simulation of the geometry of the system in the absence of the electron beam.

We also simulated the primary electron beam of 100 MeV located in a 10 degrees cone and at -10cm from the position of the water molecules along the z axis.

The following Fig. 2 shows the trajectories (traces) of the electrons given by the simulation for the incident electron beam of 100 MeV after the impact of electron collision on liquid water molecules

3.1 Linear Energy Transfer (LET)

A charged particle penetrating a given medium interacts with the atoms of the medium and undergoes a slowing down. Throughout its journey, the particle is subjected to a series of interactions during which it transfers part of its energy to the material until it comes to a complete stop in it (thermalization). One of the concrete ways to quantify this energy transfer is given by a physical quantity called the Linear Energy Transfer (LET). LET represents energy average transferred to the material per unit length of particle trajectory and is often expressed in MeV/cm. The LET is therefore equal to $\frac{dE}{dx}$ and depends on several characteristics of the particle (its energy, its mass number, its atomic number) or even on the medium it passes through.

The values of the LET, of the simulation by impact of electrons on the liquid water molecules, which we obtained are represented on the Graph 1. The LET representation of the impact of electrons on water molecules as a function of incident electron energies that we made using the root software.

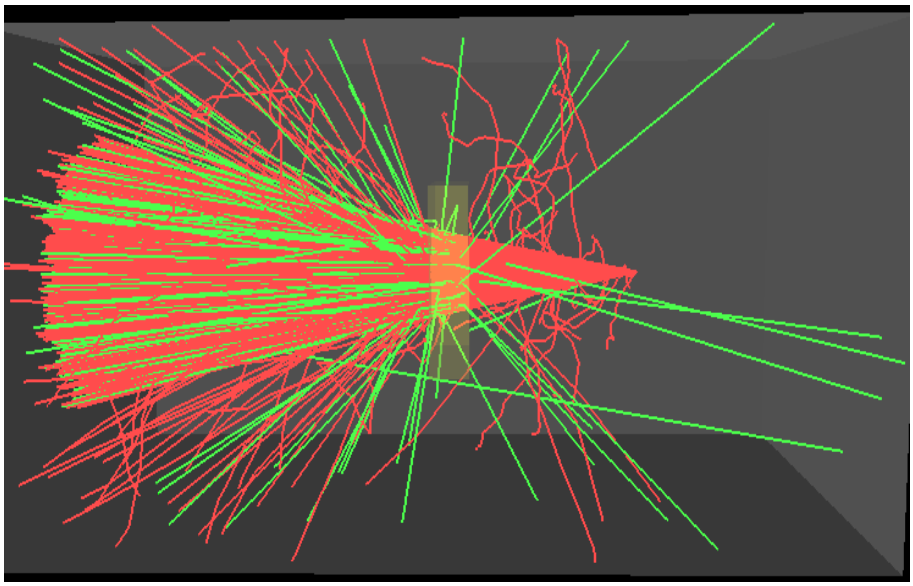
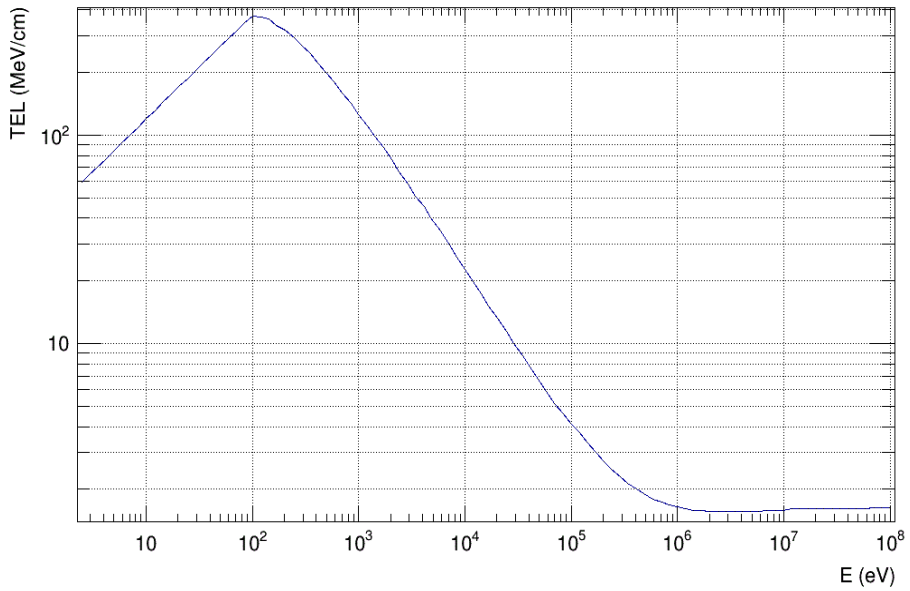


Fig. 2. Geometry, side view, following the impact of the electron beam in GAMOS



Graph 1. Linear Energy Transfer (LET) representation curve as a function of incident electron energy

This curve was plotted using the LET data that we obtained with the GAMOS software; it reaches its maximum around 37.0626 MeV/mm for an energy of 102.447 eV of the incident electrons corresponding to an average free path, in liquid water, of 2.764 nm. It decreases gradually to reach an average value of 0.161744 MeV/mm around 100 MeV corresponding to an average free path of 6.18 cm.

The LET and the mean free path in water being inversely proportional; the lower is the TEL that means the mean free path increases. The value of 6.18cm may correspond to the path of electrons outside the volume of liquid water corresponding to the path of high energy electrons and therefore there was less interaction with liquid water.

It can be seen that the values of the LET are much greater at low energies (less than 1 MeV).

Thus for low-energy and therefore low-speed electrons, they lose much more energy as they travel through the water liquid, so the TEL becomes important.

On the other hand, the LET becomes weak and tends towards an asymptotic value at high energies (beyond 1 MeV).

So high-energy and therefore high-speed electrons lose less energy in their journey through matter.

This curve therefore increases between 2.5 eV and 102.447 eV corresponding to a range of increased energy losses of electrons in favor of the medium crossed because of the low energies of the incident electrons. Then this curve decreases from 102.447 eV to 1 MeV corresponding to a gradual decrease in energy loss of the incident electron.

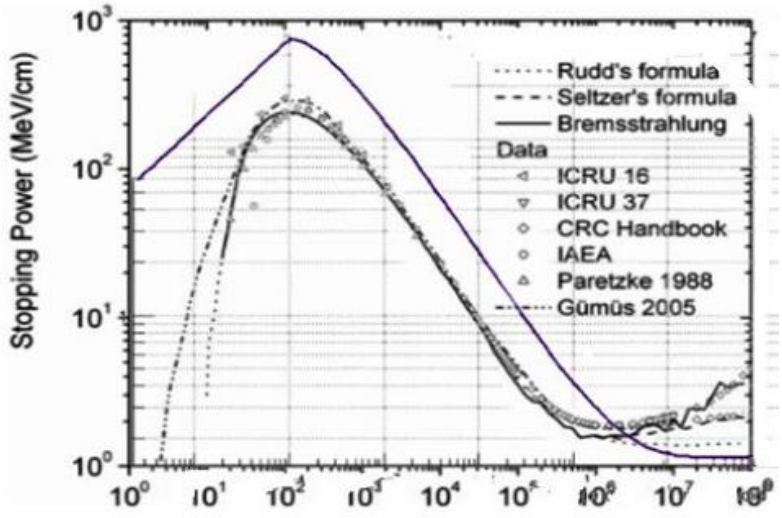
Thus, the greater the energy of the incident electrons, the less there is loss of this energy.

Finally, this curve becomes practically constant beyond 1 MeV corresponding to the high energy range of the incident electrons.

NOTICED

- The greater the energy of the incident electrons, the less there is loss of this energy and vice-versa.

This tendency is observed in the calculation made by Gümü [16]; Paretzke [17]; The same is true for the stopping power data in the CRC manual [18]; Watt et al. [19]; ICRU 37 [20]; ICRU 16 [21]; and AIEA [IAEA, 1995]; the TEL calculated by RETRACKS with the formulas of Rudd and Seltzer, with and without Bremsstrahlung [22].



Graph 2. Overlay and comparison of our graph and those of other TEL graphs

For most of these data, the plotted curves all have a maximum around 37.0626 MeV/mm for an incident electron energy of around 102.447 eV. They decrease between 102.447 eV and 1 MeV. This corresponds exactly to the behavior of the curve drawn from our simulation data.

The curve resulting from our data is above the other curves for electron energy values lower than 1 MeV. Moreover, it is below all the other curves for electron energy values greater than 1 MeV

A certain divergence appears beyond 1 MeV between our results and the other data except for the case of the Rudd formula whose data have the same trend as our data.

There are significant differences between the simulated curves and other literature. These differences can be due to the fact that our simulation overestimates the result for low energies and underestimates the results for high energies.

4. CONCLUSION

During this simulation, we analyzed the behavior of the LET as a function of the energies of the incident electrons and we compared the results obtained with experimental data and those in the literature. It appears that there is an excellent agreement of our simulation with these existing data.

The greater the energy of the incident electrons, the less there is loss of this energy and vice versa the loss of energy is greater when the energy of the incident electrons is low.

This study allowed us to confirm the hypothesis that the greater the energy of the incident particles, the less there is loss of this energy and vice versa the loss of energy is greater when the energy of the incident particles is low.

COMPETING INTERESTS

Authors have declared that no competing interests exist.

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