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Secondary electron Production by Protons and α Particles in Water Targets in the Dielectric Approximation

B. M. Magiore[1], J. G. Ternes[2],
V. R. da Silva[3] and J. Mesa[4]

[1] *beatriz.magiore@unesp.br, Department of Biophysics and Pharmacology, IBB-UNESP, Botucatu, Brazil.*
[2] *j.ternes@unesp.br, Department of Biophysics and Pharmacology, IBB-UNESP, Botucatu, Brazil.*
[3] *victoria.raposo@unesp.br, Department of Biophysics and Pharmacology, IBB-UNESP, Botucatu,Brazil.*
[4] *joel.mesa@unesp.br, Department of Biophysics and Pharmacology, IBB-UNESP, Botucatu, Brazil.*

1. Introduction

If any kind of ionizing radiation is absorbed by biological material, there is a possibility that it will interact with critical areas of the cell (eg. DNA). The atoms or molecules in this region can be excited or ionized, and thus start the sequence of events that will lead to biological effects. This type of interaction is called direct action of radiation, and it is the dominant process in high LET (Linear Energy Transfer) radiation, such as neutrons or α particles. On the other hand, radiation can interact with atoms/molecules that are outside critical regions of the cell, producing free radicals, and these will attack the DNA. This is called the indirect action of radiation, and it accounts for 2/3 of cell death and DNA damage. Because the cell is composed of 70 to 80% of water, when the radiation passes, it leads to the production of free radicals (eaq, H^+, ^-OH) and molecular forms (H_2, H_2O_2)[1]. The present work aims to study the energy transferred to H_2O targets by proton beams and α particles for further calculation of the production efficiency of ^-OH and H^+ radicals. The calculation was implemented using the dielectric approximation. The stopping power and the inverse of the mean free path, essential ingredients for this type of calculation, were obtained using the dielectric approximation. Additionally, it was possible to calculate the average energy transferred by projectiles of different energies to the target, as a measure of the production efficiency of electronic excitations and ionizations. This result will serve to estimate the probability of indirect damage caused by radiation on DNA.

2. Methodology

The dielectric formalism[2] provides the expressions to calculate the statistical moments of the energy loss distribution of an energy particle that interacts with a material medium, according to Eq. 1:

$$\frac{2}{\hbar\pi v^2}\int_0^\infty dk\,\frac{\rho_q^2(k)}{k}\int_0^{kv}(\hbar\omega)^{\mathrm{n}}\,\mathrm{Im}\left[-\frac{1}{\varepsilon(\mathrm{k},\omega)}\right]d\omega = \begin{cases} \lambda^{-1} & \text{if } n=0 \\ S & \text{if } n=1 \\ \Omega^2 & \text{if } n=2\,. \end{cases} \tag{1}$$

In this equation, v is the velocity of the projectile, $\hbar\omega$ and $\hbar k$ are, respectively, the energy and momentum transferred in an inelastic collision, $\rho_q(k)$ is the Fourier transform of the electronic density of charge q of the projectile, and $Im\left|-\frac{1}{\varepsilon(k,\omega)}\right|$ is the energy loss function (ELF) of the target, obtained from the dielectric function $\varepsilon(k,\omega)$.

In this sense, the zero moment (n = 0) corresponds to the inverse of the mean inelastic free path (λ^{-1}) which is related to the cross section σ for an inelastic event like $\lambda^{-1}=N\sigma$ where N is the density of centers of target spread. The first moment (n = 1) is the average loss of energy per unit of distance traveled, which coincides with the stopping power S. The stochastic fluctuations in energy loss by the projectile are considered by the second moment (n = 2), that defines the dispersion in energy loss, known as straggling Ω^2

The state of charge q of a projectile, with the atomic number Z_1, and moving through a condensed medium, can vary due to electron capture and loss processes. Thus, for low and intermediate projectile energies, these dynamic charge exchange processes happen continuously along the projectile's path through the target, affecting the way in which energy is lost. When charge balance is reached, usually $\sim 10^{-13}$ s after the projectile begins to penetrate the target, the magnitudes associated with energy loss can be obtained from a sum weighted by the corresponding charge state q, given by Eq. 2:

$$\begin{aligned} \Lambda\mathrm{p}(E) &= \sum_{q=0}^{Z_1} \varphi_q(E)\lambda_q^{-1}(E) \\ Sp(E) &= \sum_{q=0}^{Z_1} \varphi_q(E)S_q(E) \\ \Omega^2(E) &= \sum_{q=0}^{Z_1} \varphi_q(E)\Omega_q^2(E) \end{aligned} \tag{2}$$

where $\varphi_q(E)$ is the probability of finding the projectile with a given charge q at energy E. The sums in the previous equations extend over all possible states of charge q of the projectile (for proton we have two states and for α-particle, three). In equilibrium, we assume the state-of-charge fractions as dependent on the nature of the target, the type of projectile and its energy.

From these magnitudes and to assess the possible damage induced in biological materials due to irradiation with energetic particles, we can calculate the average energy transferred $W_{av}(E)$ by a projectile of energy E to the target where it produces electronic excitations and ionizations, given by Eq. 3:

$$W_{\mathrm{av}}(E) = \frac{S(E)}{\Lambda(E)} = \frac{\sum_{q=0}^{Z_1}\varphi_q(E)S_q(E)}{\sum_{q=0}^{Z_1}\varphi_q(E)\lambda_q^{-1}(E)}\,. \tag{3}$$

3. Results and Discussion

We calculated the inverse of mean free path and the stopping power of protons and α-particles in a liquid water target. With these calculations it was able to generate the graphics shown in Fig. 1 and 2, where both magnitudes were plotted as a function of E/A.

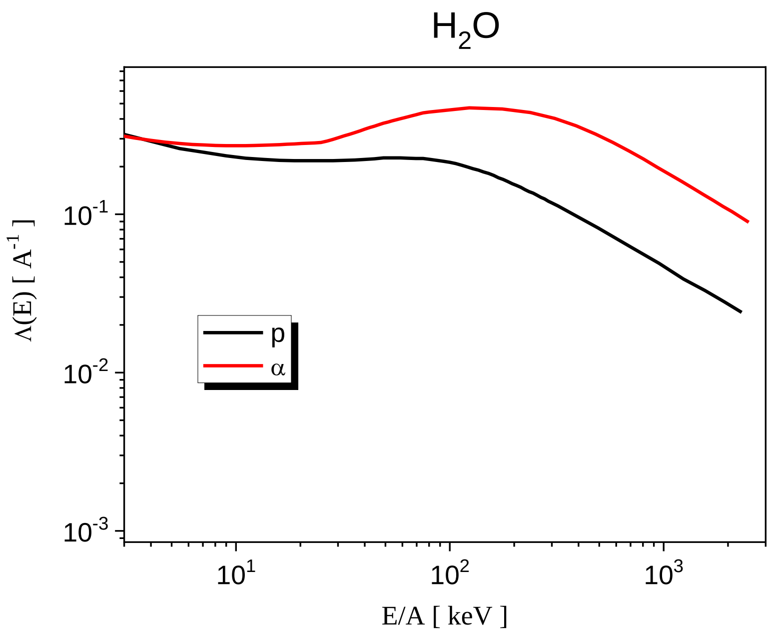

Fig.1: Inverse of the mean free path (Λ) as a function of the incident particle energy (E/A).

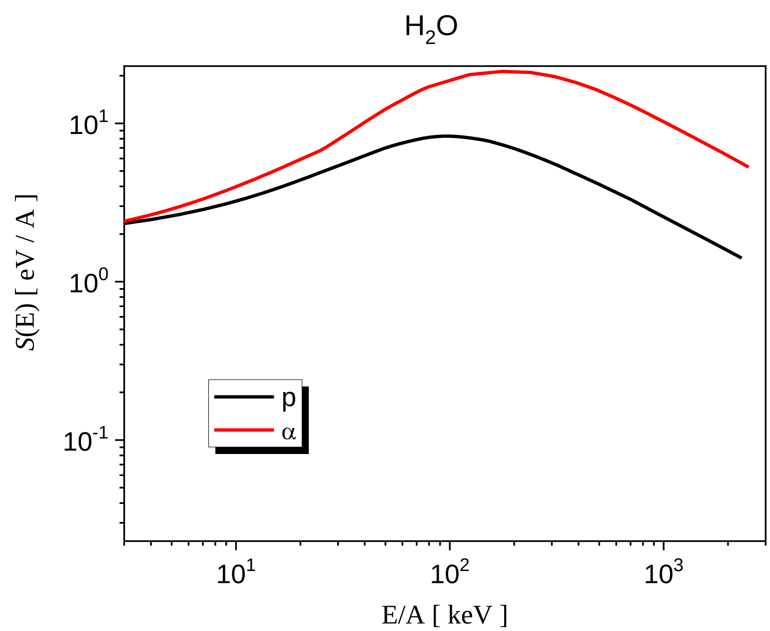

Fig. 2: Stopping power (*S*) as a function of incident particle energy (E/A).

The calculated stopping powers and the inverse of the mean free paths were greater for the α–particle: therefore, the charge of the α–particle is twice that of the proton, its interaction capacity is greater, resulting in higher energy deposition in each interaction and in smaller distances between two consecutive interactions. Despite these differences, and as can be verified in Fig. 3 for the range of energies studied, the mean energy transfer to electrons by inelastic processes has a similar behavior for the two particles, being slightly higher for α-particles.

As it is well known, E_{lig} ~ 10 *eV* for most biomaterials. Consequently, the secondary electrons produced in water by protons and α-particles with E/A > 10 keV have enough energy to start causing radiolysis efficiently. As the results obtained in this work were established from first principles, it will be possible to establish through them more reliable and closer to real values of linear energy transfer (LET), deposited dose and radiobiological effectiveness (RBE) for ions in biomaterials.

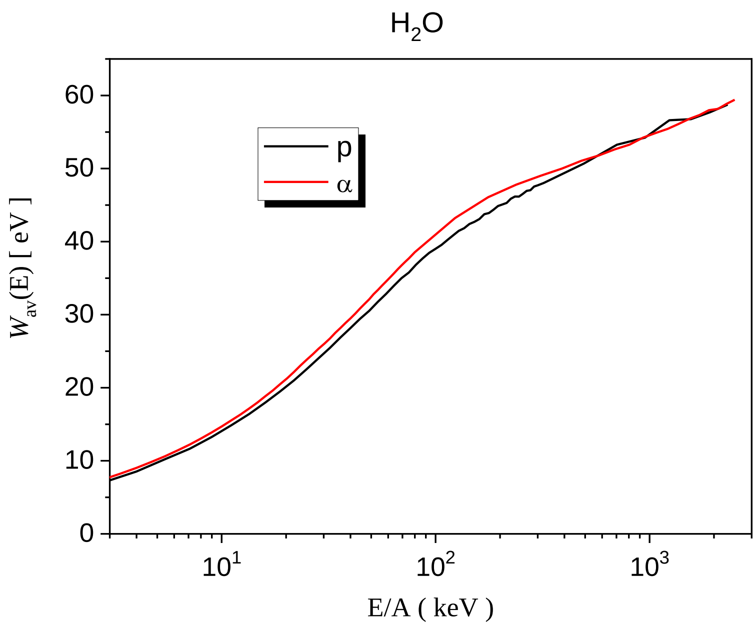

Fig. 3: Average energy transferred for electrons (W_{av}) as a function of the incident particle energy (E).

4. Conclusions

The dielectric formalism allowed to perform a satisfactory calculation of the average energy transferred by an ionic projectile in H_2O. The next steps, already in progress, include the implementation of the calculation of the inverse of the mean free path and the stopping power, as well as the yield of secondary electrons and its energy spectrum employing the Monte Carlo codes SRIM[3] and FLUKA[4] to compare and validate the results.

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