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Theoretical study of W-values for particle impact on water

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ABSTRACT

The *W-values* and the differential values *w,* were calculated by electron, proton and antiproton impact on liquid and vapor water. Two different theoretical approximations were used: the Fowler Equation (based on the Continuous Slowing Down Approximation), and the Monte Carlo code MDM, which does an event-by-event tracking of all generated particles in the media. The dependence on the type and charge of the projectiles and the relevance on the appropriate inelastic cross sections employed in the calculations were studied. For electron impact, results obtained with both models are in good agreement with experimental data and with other theoretical calculations. However, the MDM results are more representative of the stochastic nature of radiation-media interactions. The *w*-values for swift proton and antiproton impact on vapor water, calculated using the Fowler Equation, are in very good agreement with the results obtained by electron impact in the same velocity regime.

1. Introduction

The *W-value* is a quantity widely used in radiation physics (dosimetry, medical physics, astrophysics). It corresponds to the mean energy required to generate an ion-electron pair (electron – ionized molecule or atom) upon the complete slowing down of the ionizing radiation. This parameter is precisely defined as the ratio between the kinetic energy *T* of the incident particle and the average number of ion-electron pairs *N* formed upon the total dissipation of the kinetic energy of the primary particle and that of all the secondary electrons produced by ionization processes

$$W = T/N \tag{1}$$

The *W-values* depend on the atomic or molecular composition of the target. This dependence is based on the cross sections of the inelastic processes in radiation-matter collision. Generally, these cross sections depend on the energy and charge of the projectile. In the case of electron, proton and antiproton impact at intermediate and low velocities, the inelastic cross sections are very different. However, at high impact velocities, the ionization cross sections converge to the same values [1]. Therefore, it is expected that in the high impact velocity regime the *W-values* for proton, antiproton and electron impact would converge to the same values. Indeed, it has been observed experimentally that this parameter has an asymptotic behavior at high velocities [2]. The almost constant value of *W* in the asymptotic limit is the base on which the experimental dosimetry is supported [3].

Ionization chambers filled with air are used in reference dosimetry to determine the dose delivered. The measurement of all the liberated charges (mainly secondary electrons) in the ionization chamber is related with the dose through the *W-values*. The presence of water vapor (air humidity) can influence the cavity measurements and must be considered. The uncertainties in the *W-values* affect directly the dose determination. In the case of proton therapy and hadrontherapy the *W-values* are the most important source of uncertainties in reference dosimetry [4]. Therefore, research in this field is of fundamental interest.

In the case of high energy particle impact in a thin media (ionization chamber), only a small fraction of its energy is lost, therefore the differential *w-value* should be employed. It is defined on a small segment of the projectile track, in which the inelastic collision cross sections are almost constant. It is calculated as the ratio between *dT*, the average energy lost by a particle (with initial energy *T)* when traveling through a thin thickness of a medium, and *dN* the average number of ion-electron pairs produced by dissipating totally that differential energy in the medium,

$$w = dT/dN \tag{2}$$

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The differential *w-value* is related to the *W-value* as follows:

$$\frac{1}{w(T)} = \frac{d}{dT}\left(\frac{T}{W}\right) \tag{3}$$

In the limit of high-energy impact, where the *W-values* are almost constant, $w \equiv W$. This characteristic is used in dosimetry for hadrontherapy to establish the reference value [4].

Experimental *W-values* for electron and ion impact (proton and alpha particles) on some gases have been measured for energies up to the asymptotic limit (over 10 keV for electrons and 10 MeV/u for ions), but which are small compared with the energies required for radiotherapy [2]. For the case of electron impact on vapor water, there are experimental data from Combecher (1980) [5] and from Christophorou (1971) [6]. The measured value of 29.6 ± 1 eV in the asymptotic limit [6] was adopted as a reference value by ICRU REPORT 31 [3]. For liquid water, a limit value of 22 ± 1 eV is proposed taking into account the radiolytical yields of solvated electrons and other spurs after 1 MeV electron irradiation (Mozunder and Hatano (2004) [7] and references there in). The smaller value for the liquid phase of water could be related to the increase in the ionization probability by the modification of the ionization potential and the interaction of excited molecules with their neighbors (Mozunder (1999) [8]). In a recent article [9], *W-values* for electron impact on liquid water was calculated using the GEANT4-DNA, as a benchmark for the election of the most representative cross sections for inelastic processes. For proton and other ion impact, there are not experimental data in vapor and liquid water to compare with. Therefore, theoretical calculations are required to extend the results to additional particle beams and energy range. Currently, different approximations to calculate the *W-value* for electron and ion impact exist. Regarding the bookkeeping problem in transport theory, there are several models with the basis of the continuous slowing down approximating where an integral equation for the energy distribution of all the electrons is used. For electron impact a semi-analytical theory was developed by Spencer and Fano [10]. It is described as an integral equation related to the total path-length of all the electrons in the media. There is also a recursive equation, called the Fowler equation [11], which we shall describe in the next section.

In the case of ion impact, it is possible to generated new species as projectiles due to the ion-matter interaction, e.g. charge exchange. Therefore, the ion-electron pair counting should be calculated for each of these processes [12].

In the present work, the differential *w* and *W-values* for electron, antiproton and proton impact on vapor water were calculated. To obtain these parameters, *inelastic cross sections* and the *cumulative counting* of all the inelastic processes induced by the incident and secondary particles were necessary. The main inelastic cross sections considered were the ionization and electronic excitation. For the cumulative counting processes, we used two models: The *Fowler Equation (FE),* which is a recursive equation developed by Inokuti (1975) [11], based on the Continuum Slowing Down Approximation (CSDA), and the Monte Carlo code MDM developed by Gervais et al. [13,14]. The MDM code enables to track the history, event-by-event, of all the particles (the primary projectile and all the secondary electrons generated by ionization of the target molecules) down to thermalization energy.

2. Methods

2.1. Cumulative counting models

2.1.1. Fowler equation

Within a continuous slowing down approximation (CSDA) the *w-values* for the case of a single charge state (i.e. by electron or antiproton impact where the electron capture is forbidden) can be calculated using the following equation (Erskine (1954) [15]; Dalgarno and Griffing (1958) [16]):

$$w(T) = \frac{\epsilon(T)}{\sigma_{ion}(T) + \sigma'_{ion}(T)} \tag{4}$$

where ϵ is the stopping cross section, σ_{ion} is the ionization cross section and σ'_{ion} is the cross section associated with the production of an ion-electron pair by secondary processes. If only the primary ionization process is considered, the previous expression takes the form,

$$w_{prim}(T) = \frac{\epsilon(T)}{\sigma_{ion}(T)} \tag{5}$$

The cross section for secondary processes is defined as:

$$\sigma'_{ion}(T) = \sum_i \left[\int_{E_{min}}^{E_{max}} \frac{d\sigma_i^{ion}}{dE} J(E)dE \right] \tag{6}$$

$d\sigma_i^{ion}/dE$ being the simple differential cross section of ionization for each molecular or atomic orbital *i* as a function of the energy of the ejected electron *E,* and the function *J*(*E*) being the average number of ion-electron pairs produced by the ejected electron after total dissipation of their kinetic energy *E*. To determine, *J*(*E*) we used the generalized *Fowler Equation* [11],

$$\begin{aligned} J(E) &= P_{ion}(E) + \textstyle\sum_n P_n^{exc}(E) J(E - E_n^{exc}) \\ &+ \textstyle\sum_k \left[\int_{E_{min}}^{(E-B_k)/2} dE' \frac{d\sigma_k^{ion}}{dE'} \frac{1}{\sigma_T(E)} \{J(E - E' - B_k) + J(E')\} \right] \end{aligned} \tag{7}$$

with $P_{ion}(E) = \sum_k \sigma_k^{ion}(E)/\sigma_T(E)$; where σ_k^{ion} is the total cross section of the k-molecular orbital ionization by electron impact and $\sigma_T(E) = \sum_n \sigma_n^{exc}(E) + \sum_k \sigma_k^{ion}(E)$, where σ_n^{exc} is the cross section to excite the water molecule to a discrete level n transferring an energy E_n^{exc}. $P_n^{exc}(E) = \sigma_n^{exc}(E)/\sigma_T(E)$ and we define the probability to produce a secondary electron of energy E' from the orbital k by impact of an electron of energy E as $\frac{d\sigma_k^{ion}}{dE'}\frac{1}{\sigma_T(E)}$. B_k is the binding energy of the k-molecular orbital.

The stopping cross section for the case of electron impact was calculated using the expression:

$$\epsilon(T) = \sum_n \sigma_n^{exc} \Delta E_n + \sum_i \left[\int_{E_{min}}^{E_{max}} \frac{d\sigma_i^{ion}}{dE} (E + B_i) dE \right] \tag{8}$$

where ΔE_n, and $E + B_i$ represents the energy transferred by the projectile in the process of excitation and ionization respectively.

In the case of proton impact, the electron capture process must be considered for impact energies smaller than 500 keV approximately on liquid or vapor water [17]. After electron capture the proton projectile is transformed into a neutral hydrogen atom, then the beam is integrated by two different states of charge in equilibrium. This effect contributes to the stopping power as follow:

$$S = f(H^+)S^+ + f(H^0)S^0 \tag{9}$$

where $f(H^+)$ and $f(H^0)$ represent the charge fraction of protons and hydrogens integrating the beam and $S^+$and S^0 the corresponding stopping powers. However, for impact energies over 500 keV the contribution of the neutral fraction can be neglected [17].

For electron and proton impact we do not need to consider elastic-collision cross sections because the energy loss upon an elastic collision with any molecule is negligible.

2.1.2. Monte Carlo simulation

In Monte Carlo simulation of radiation transport, the history (track) of a particle is viewed as a random sequence of free flights that ends with an interaction event where the particle changes its direction of movement, loses energy and, occasionally, produces secondary particles. In a homogeneous medium, the flight distance between two successive collisions or step length *s* obeys the Poisson probability distribution. It is sampled according to,

$$s = -\lambda_T \ln\xi \quad (10)$$

where ξ is a random number uniformly distributed in the range of (0,1] and λ_T is the total mean free path defined as $\lambda_T^{-1} = \sigma_T n$ with σ_T the total collision cross section and n the molecular density of the medium. A detailed description of the MDM code for liquid water can be found in Gervais et al. (2006) [13,14]. For the case of vapor water, we will present them in the next Sections (3.1 and 3.2).

We associated the number of ion-electron pairs *N* with the number of electrons generated in the MDM simulation, after the interaction of the primary and secondary particles with the molecules of the medium through different inelastic processes. All the generated electrons are followed down to thermalization, i.e. down to sufficiently low energy to ensure that all ionization processes are exhausted. Thus, the *W-values* as a function of the incident energy is obtained as the initial particle energy divided by the number of created electrons (*T/N*).

2.2. Inelastic cross sections

2.2.1. Electron projectile

The case of electron impact is of relevance for all type of ionizing radiation: secondary electrons produced after ionization processes are responsible for energy deposition. Experiments in water vapor by electron impact were conducted to determine the total ionization cross sections and the single differential values as a function of the emitted electron energy [18,19,20], and some semi-empirical models based on these measurements were developed [21,22]. For our calculations on water we implemented the BEB model (Binary-Encounter-Bethe) of Kim and Rudd (1994) [23]. This model combines the binary-encounter theory with the dipole interaction of the Bethe theory for fast incident electrons. It is fairly accurate to describe the ionization and it is not limited to the high energy range as the first-Born approximation. The ionization energies used in our calculations are shown on Table 1.

In the case of electronic excitation cross sections, we used the semi-empirical equation proposed by Green and Stolarsky (1972) [24]. We considered five electronic excited states for water molecule (see Table 2). The vibrational excitation cross sections and dissociative excitation processes were also calculated using the same semi-empirical function for vapor water (Olivero et al. (1972) [25]). The energies considered for the nine vibrational states and the three dissociative excitations states are given in Table 3.

2.2.2. Proton projectile

Inelastic experimental cross sections by proton impact on water are scarce, especially for the excitation processes. Theoretical total ionization cross section and electron capture cross section were calculated applying the continuum distorted wave-eikonal initial state (CDW-EIS) approximation, used successfully to study different targets interacting with ion projectiles [29,30,17]. Ionization cross sections were calculated also with the semi-empirical model of Rudd [31]. Excitation cross sections were calculated extending the Green and Stolarsky electron model to the case of protons using a speed scaling, since for high impact velocities these cross sections converge to the same values according to the first Born theory. This straight forward scaling is defined by,

Table 1
Ionization energies for vapor and liquid water from Hwang-Kim-Rudd (1996) [26] and Dingfelder et al. (1998) [27].

Target	i	Molecular orbitals	E_i (eV)	
			Liquid	Vapor
H_2O	1	$1a_1$	539.0	539.7
	2	$2a_1$	32.3	36.88
	3	$1b_2$	16.05	19.83
	4	$3a_1$	13.39	15.57
	5	$1b_1$	10.79	12.61

Table 2
Excitation energies for vapor and liquid water from Emfietzoglou et al. (2000) [28].

Target	n	Excitation state	E_n (eV)	
			Liquid	Vapor
H_2O	1	A^1B_1	8.4	7.4
	2	B^1A_1	10.1	9.67
	3	*Rydberg A + B*	11.26	10.0
	4	*Rydberg C + D*	11.93	11.06
	5	*Diffuse Band*	14.1	13.32

Table 3
Vibrational and dissociative excitation energies for vapor water from Olivero et al. (1972) [25].

Target	n	Vibrational States	E_n (eV)
H_2O vapor	1	ν_2	0.195
	2	$2\nu_2$	0.391
	3	$\nu_1(1\,0\,0)$	0.453
	4	$\nu_3(0\,0\,1)$	0.466
	5	$\nu_2 + \nu_3$	0.661
	6	$\nu_1 + \nu_3$	0.899
	7	$\nu_1 + \nu_2 + \nu_3$	1.092
	8	$2\nu_1 + \nu_3$	1.316
	n	Dissociative states	E_n (eV)
H_2O vapor	1	*H* Lyman α*	17.0
	2	*H* Hα*	19.0
	3	*OH*, 3064 A*	10.0

$\sigma_{exc}^{proton}(Tp) = \sigma_{exc}^{electron}(T)$, with $T = Tp(me/mp)$ where m_e and m_p are their masses respectively.

3. Results and discussions

3.1. Electron projectile

The set of electron collision cross sections used in the MDM and FE simulations for vapor water are shown in Fig. 1. The vibrational cross sections decrease sharply reaching too small values at an incident electron energy of 10 eV. The ionization dominates in the range of intermediate and high energies against the excitation process.

In Fig. 2, we plotted the mass stopping power S_{mass} for electron impact in vapor water. To obtain these values we used the relation:

$$\epsilon(T) = 10^{21}\left(\frac{M_m}{N_A}\right) S_{mass}(T) \quad [10^{15} eV cm^2] \quad (11)$$

where $\epsilon(T)$ is the stopping cross section calculated using Eq. (7). M_m is the molar mass of the media and N_A Avogadrós number. These values are compared with data from NIST [32], ICRU REPORT 16 [33] and IAEA TECDOC-799 [2], showing good agreement for energies above 1 keV. The data dispersion is appreciable in the low and intermediate energy range.

In Fig. 3 we show the number of ion-electron pairs obtained applying the FE and MDM models described in the previous section. This function seems to be lineal above 100 eV for the electron impact energy.

The calculated *W-values* for electron impact in vapor water with both theoretical models are shown in Fig. 4, compared with experimental determinations from Combecher (1980) [5] and another empirical calculation from Inokuti (1975) [11]. We can notice a good agreement in the region of intermediate and high energies, especially in the asymptotic limit where the two models, FE and MDM, reach values close to 29.6 eV measured by Christophorou et al. (1971) [6] and adopted by ICRU REPORT 31 [3] as a reference value.

The most sensitive energy range for the *W-values* is below approximately 50 eV. However, the lack of experimental data in the

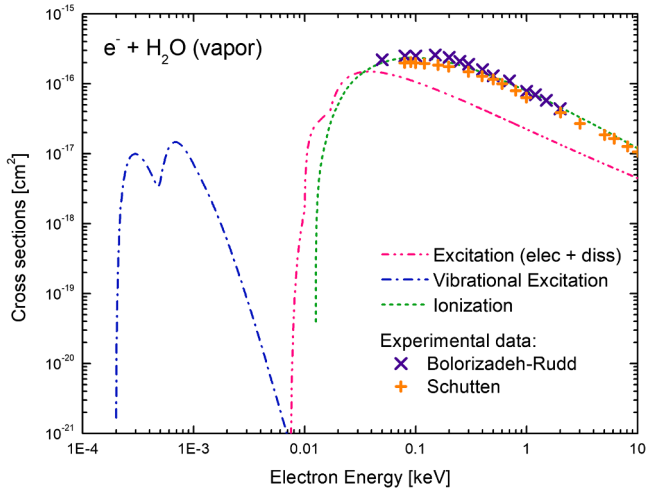

Fig. 1. Inelastic cross sections for electron impact in vapor water as a function of incident electron energy. The sum of the excitation cross sections from Green and Stolarsky (1972) [24] and the dissociative excitation cross section from Olivero et al. (1972) [25] is represented with dash-dot-dot pink line. Total vibrational excitation cross section is from Olivero et al. (1972) [25] with dash-dot blue line. Total ionization cross section from Kim and Rudd (1994) [23] is represented with dash green line. They are compared with experimental data from Shutten et al. (1965) [19] and Bolorizadeh and Rudd, (1986) [20]. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

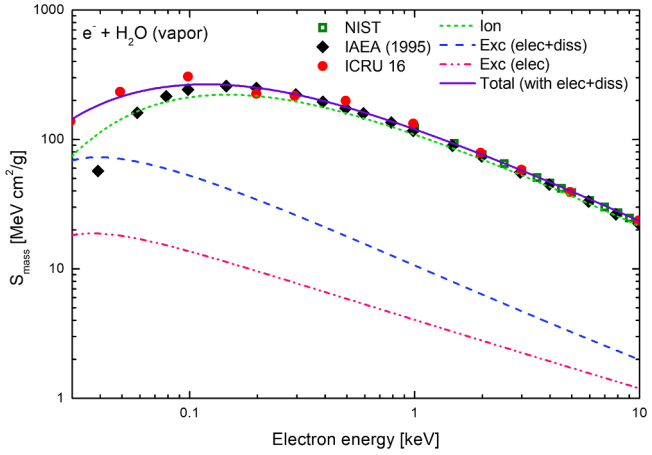

Fig. 2. Mass stopping power for electron impact on vapor water. The contributions of the ionization and excitation processes are analyzed. Recommended and experimental values are presented from NIST [32], IAEA [2] and ICRU 16 [33].

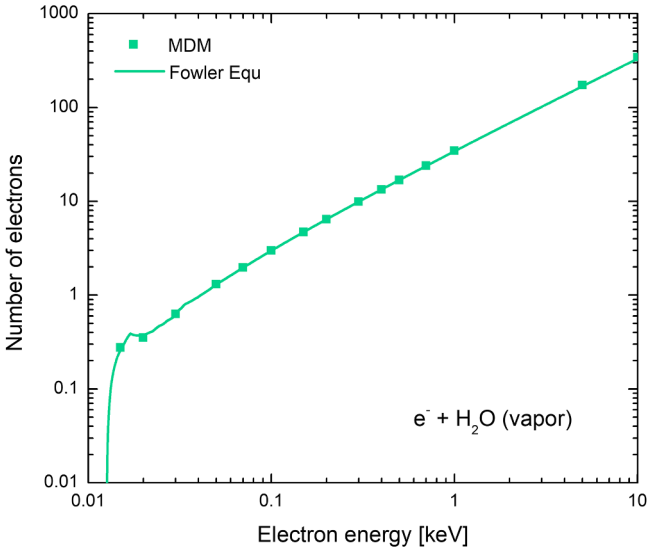

Fig. 3. Number of ejected electrons per incident electron calculated with both models, Fowler Equation (solid line) and MDM code (square) in vapor water versus the incident electron energy.

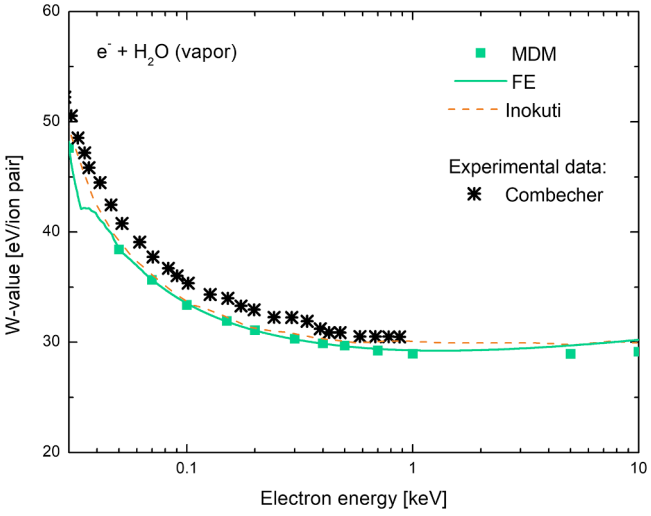

Fig. 4. W-values for electron impact in vapor water as function of incident electron energy. Values calculated with Fowler equation (solid green line) and MDM code (square) are show and compared with experimental data from Combecher (1980) [5] (star) and a theoretical calculation by Inokuti (1975) [11] (dashed line). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

region of low energies for the inelastic cross sections, and thus the stopping power, impact on the accuracy of the models to calculate them and therefore affect the *W-values*.

We would like to emphasize the relevance of the inelastic cross sections used for electron impact on water vapor. In Fig. 5 we show the difference in *W-values* considering five electronic excitations states against considering also three dissociative excitation states. The *W-values* calculated with only five excitation states is about 15% lower than the measured values and thus the ones considering all the excitation states.

In the case of liquid water, a detailed description of the cross sections used in the MDM Monte Carlo code can be found in Gervais et al. (2006) [13]. In Fig. 6 we plotted the inelastic cross sections considered and also added the electronic excitation cross section calculated with the model of Green and Stolarsky (1972) [24] (see Table 1). These excitation cross sections are higher than those used by Gervais et al. (2006) [13] in almost the entire range of energy. Therefore, the probability of ionizing the molecule is lower and higher *W-values* are expected.

In Fig. 7 we can observe the *W-values* calculated applying the FE and MDM models, using the same cross section except those of electronic excitation. All of them are very close to the value 22 eV (indicated with a row), referred by Mozunder and Hatano (2004) [7] in the high energy range. They are compared with results from Monte Carlo codes PARTRAC and GEANT4-DNA [9]. *W-values* from GEANT4-DNA are closer to our calculations, PARTRAC shows an asymptotic value larger to the other calculations.

3.2. Proton projectiles

In Fig. 8 we show ionization and electron capture experimental cross sections from Rudd-Goffe and Rudd-Toburen [34]. As we can

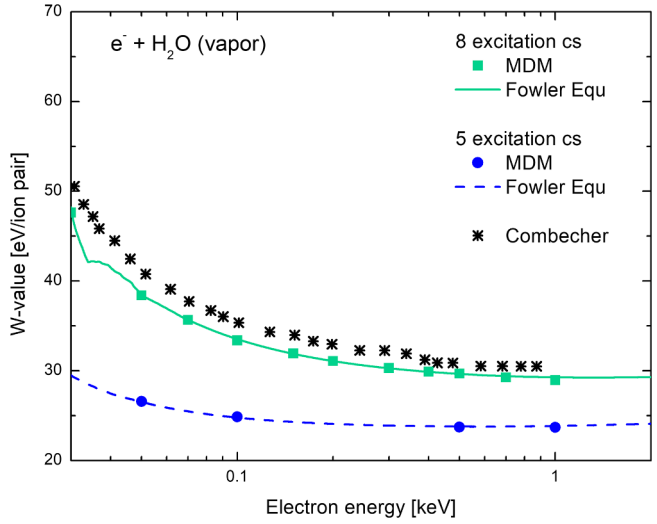

Fig. 5. W-values for electron impact in vapor water as function of incident electron energy. Values calculated with Fowler equation (solid line 8 excitation states; dash line 5 excitation states) and MDM code (squares 8 excitation states; circles 5 excitation states) are calculated considering different number of excitation states. They are compared with experimental data from Combecher (1980) [5] (star).

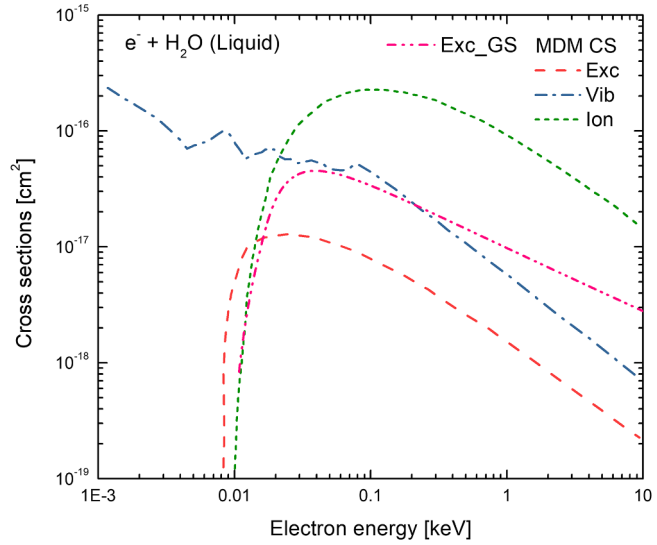

Fig. 6. Inelastic cross sections for electron impact in liquid water as a function of electron energy. Total excitation cross sections from Green and Stolarsky (1972) [24] is represented with dash-dot-dot pink line. Excitation, vibrational and ionization cross sections are from Gervais et al. (2006) [13]. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

observe for impact energy above 500 keV, the electron capture cross section is more than two order of magnitudes lower than the other processes, and it can thus be safely neglected. From this energy onwards, we considered only the contribution of protons (charge state fraction of H^+ equal to one) to the stopping power [17].

In Fig. 9 we present the mass stopping power S_{mass} for proton impact on vapor water. These values were calculated using the cross sections described in Fig. 8. We observe that the values considering the processes of ionization plus capture are closer to the recommended and experimental data in the intermediate and low energy range. The stopping power calculated with the Rudd model for ionization

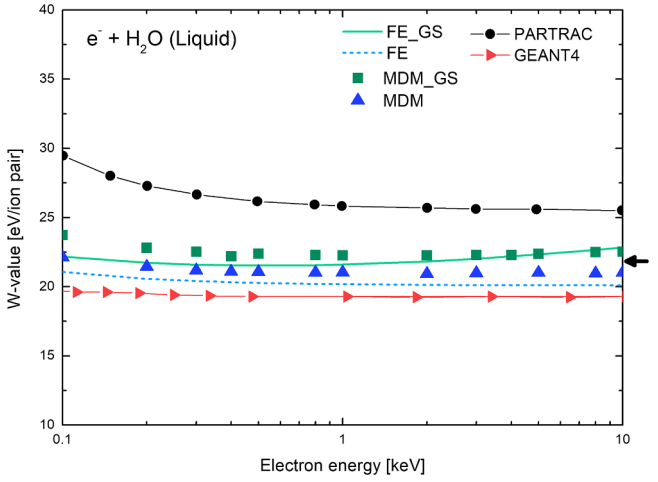

Fig. 7. *W-values* for electron impact on liquid water as a function of incident electron energy. Values calculated with Fowler equation (blue short dash line and green solid line) and with the MDM code (blue triangle dots and green square dots) are shown considering different excitation cross sections; green color refers to Green and Stolarsky and blue color refers to Gervais excitation cross sections. They are compared with simulation codes from PARTRAC and GEANT4-DNA [9]. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

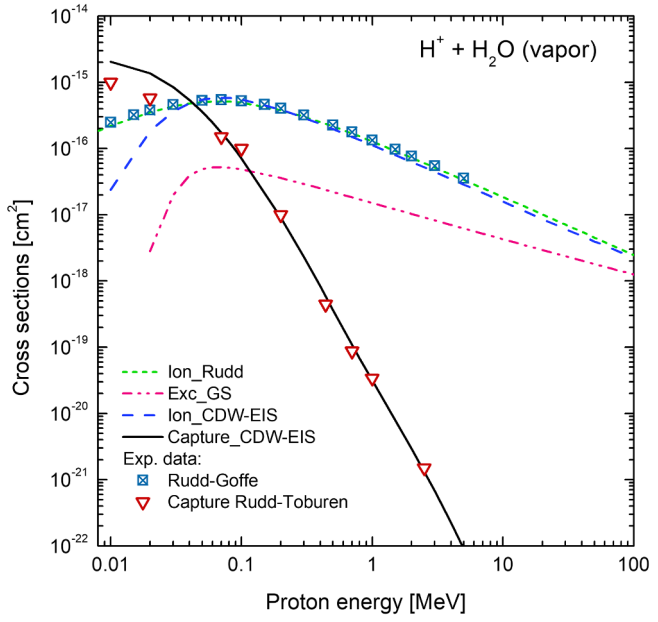

Fig. 8. Inelastic cross sections for proton impact in vapor water as function of incident proton energy. Total ionization and capture cross sections are calculated using theoretical model CDW-EIS [29,30,17] (dash blue line and solid black line) and Rudd model [31] (short dash green line). They are compared with experimental data from Rudd-Goffe and Rudd-Toburen [34]. The total excitation cross section is calculated using semi-empirical model from Green and Stolarsky (1972) [24] (dash-dot-dot line). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

converges to the values calculated with the CDW-EIS model for energies above 1 MeV.

In proton therapy, very thin ionization chambers are used for reference dosimetry and the differential *w-values* are required. In Fig. 10, the differential w and w_{prim} values for proton impact in water vapor

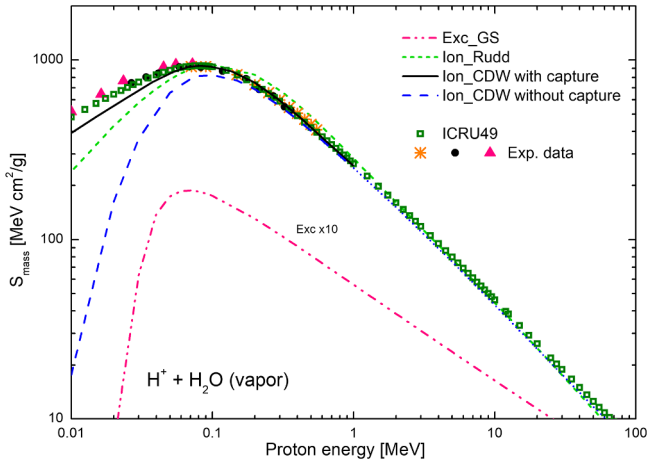

Fig. 9. Mass stopping power for proton impact on vapor water. Recommended and experimental values are taken from ICRU 49 [35] and Olivera et al. (1995) [36].

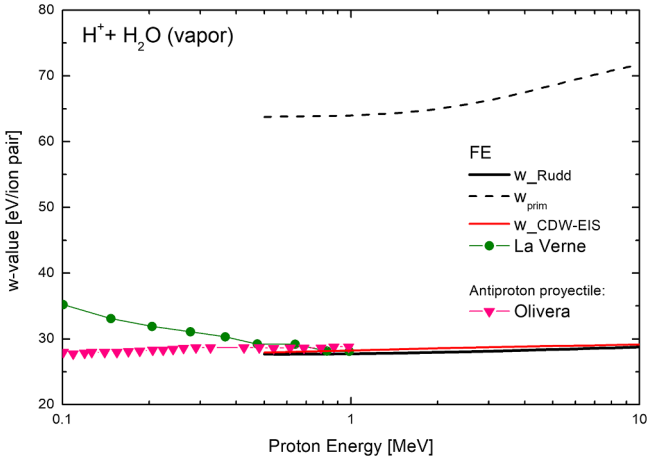

Fig. 10. Differential *w* value for proton impact in vapor water as function of proton energy. Values using Fowler Equation with different theoretical model for ionization cross sections are show: solid black line used Rudd model [31] and solid red line used CDW-EIS model [29,30,17]. This last was also calculated for antiproton projectile dash dot blue line. Values from others author are plotted to compared [37,38]. Primary *w* values were calculated using Rudd model is represented with dash black lines. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

calculated using Eqs. (3) and (4) respectively are presented. It is important to note that these values were obtained using the inelastic cross sections and mass stopping powers described above (Figs. 8 and 9), while the ionization associated with secondary electrons was obtained using the results of the previous section on electron, Fig. 3.

From our knowledge, there are not experimental data for proton impact on water to compare with. The asymptotic limit of 30.5 eV for *W-values* has been proposed by Christophorou (1971) [6]. We compare the present calculations with theoretical results from La Verne and Mozunder (1992) [37], based also on the FE and semi-empirical approximations. They took into account the charge exchange processes (electron capture and electron loss), thus their results are extended to energies smaller than 500 keV. In Fig. 10 we also present the results for antiproton impact calculated by Olivera et al. [38] for which the electron capture is forbidden. The ionization cross sections were calculated applying the CDW-EIS approximation and the excitation cross sections were extracted from Hayashi [18].

The w_{prim} value reported in Fig. 10 puts in evidence the relevance of the secondary electron contribution. The difference between this value and the w-value calculated with the full cascade of secondary electrons is as large as 50% in the high energy range. A *w-value* around 29 ± 1 eV is reached for energies above 1 MeV, which is very similar to that of electrons (29.6 ± 1 eV).

4. Conclusions

In the present work we calculated *W* and *w-values* by electron and proton impact on vapor and liquid water applying two different theoretical approaches: the FE equation (based on the CSDA) and the MDM Monte Carlo code. Both are very sensitive to the cross sections chosen to represent the inelastic interactions between the primary incident particle and all the secondary electrons with the media. The W-values for electron impact are in very good agreement with experimental values. For the case of proton and antiproton impact, the results are in good agreement with other semi-empirical results and Monte Carlo codes. These good results allow us to proceed further and extend the FE and MDM codes to calculate the *W* and *w-values* for the cases of other types of particle impact and other gases of interest in dosimetry for hadrontherapy and astrophysics.

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