

# Monte Carlo simulation of charged particle transport in biomatter

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## Abstract

Knowledge of the microscopic distribution of interactions in irradiated matter is of fundamental importance for a mechanistic understanding of subsequent effects. This may be obtained by Monte Carlo codes which simulate event-by-event the transport of charged particles in matter. The development of such codes necessitates accurate interaction cross-sections for all the important collision processes. A semi-theoretical formalism has been developed and implemented in a Monte Carlo code which fairly accurately predicts energy-loss spectra for charged particle impact on water molecules. The extension of the formalism for establishing the necessary cross-sections for liquid/solid water (i.e. more realistic biomatter) is discussed and preliminary results are presented.

KEYWORDS: Simulation, microdosimetry.

## 1. Introduction

Studying the nature of radiation induced molecular damage on biological-like materials (e.g. water) is important for understanding the pathways that lead to observable effects. This is directly linked to improved radiation protection through the use of more pertinent microdosimetric distributions, and the exercise of sounder scientific judgment. From a biophysical perspective, the fact that RBE values are usually different to one, implies that the effect depends non-linearly on the relevant stochastic quantities and thus a microdosimetric approach is necessary.

## 2. Methodology

Detailed study of charged particle tracks necessitates an event-by-event simulation of all the interactions taking place as both the primary particle and all its secondary electrons deposit their energy in matter. The interaction probabilities are described by the relevant cross-sections. For inelastic collisions the Bethe theory may be used for evaluating the probability of a given energy-transfer. For fast charged particles (keV-MeV range), it predicts that dipole interactions (soft-collisions) are dominant. On the other hand, closer collisions (approximating binary encounters) produce fast secondaries which also need to be modeled for accurate track structure study. These may be included in a semi-theoretical way after considering appropriate data for water vapor [1]. The above procedure neglects condensed-state (liquid/solid) effects arising from intermolecular interactions. To account for electronic modifications following condensation (liquid/solid environment), the energy-loss function of the condensed target needs to be known for all possible values of momentum and energy transfer.

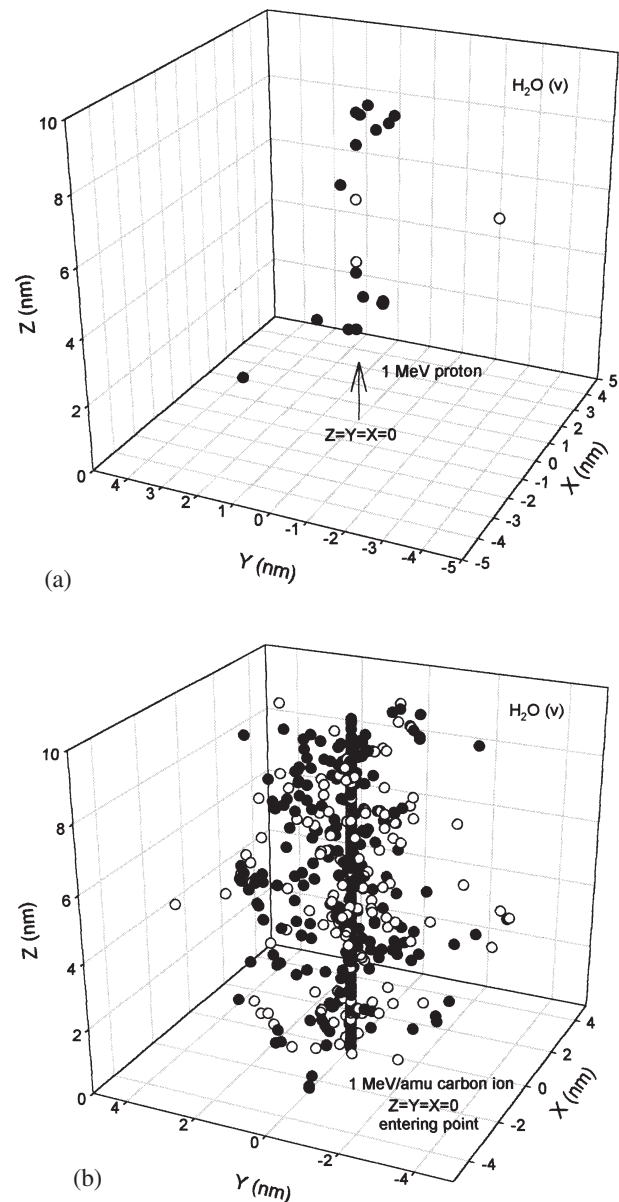


Fig. 1 – Track segments of 1 MeV/amu proton (a) and carbon ion (b). (●) ionization, (○) excitation.

### 3. Results

Figure 1 depicts simulated track segments for 1 MeV/amu proton and carbon ion. Such information along with the storage of all collision details is a prerequisite for a stochastic modeling of the physical stage of radiation action. In Figure 2 optical data of liquid water [2] have been analytically reproduced by a Drude-model. This model constitutes the basis for constructing the entire energy-loss function of liquid water. Integration of the latter over all possible momentum transfers renders inelastic cross-sections of liquid water (Fig. 3).

### 4. Discussion

The simulation of charged particle (inelastic) interactions in biological matter may be accomplished more accurately under the gas-phase approximation, i.e. neglecting intermolecular effects, due to the availability of well-established experimental data for gas targets (e.g. water vapor) [1]. Fully empirical or semi-empirical models (e.g. using Bethe's theory) may then be developed from such data [1]. In contrast, data for condensed targets are limited to the dipole limit (i.e. zero momentum transfer) obtained either from optical measurements or forward scattering experiments. To go beyond an optical data model and thus obtain more realistic inelastic cross-sections (see Figure 3) the entire energy-momentum-loss plane (the so called Bethe surface) needs to be modeled. This extension necessitates algorithms which would be sufficient accurate and at the same time computationally convenient for Monte Carlo transport codes. The results depicted in Figure 3

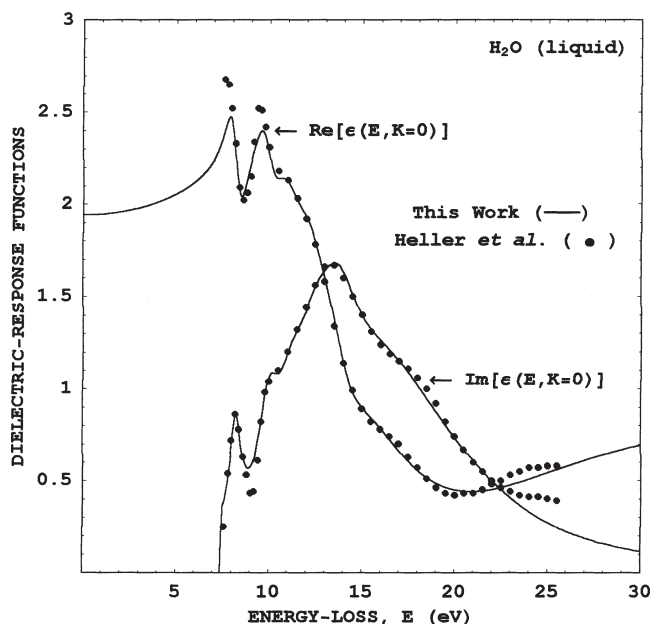


Fig. 2 – Dielectric functions of liquid water at the optical limit.

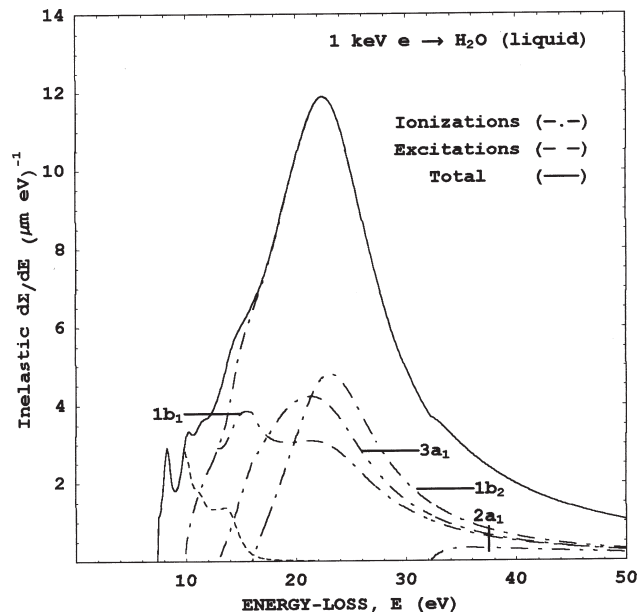


Fig. 3 – Inelastic cross-sections of liquid water differential in energy loss for 1 keV electron impact.

were obtained by a simple generalization of the dielectric response function under the constraint of a binary behavior at the limit of high energy-and momentum-loss (the so called Bethe ridge). Towards the development of an accurate data basis on inelastic cross-sections for biological materials (liquid-crystalline water, DNA) an examination of the effect of the various assumptions on the model cross-sections is under way. It is envisioned that such an effort would also benefit the accuracy of macroscopic Monte Carlo transport codes by extending the applicability of the straggling distributions to lower impact energies and/or smaller transport steps.

### Acknowledgments

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