Contribution ID: **47**

Type: **Oral**

Covering the upper clinical energy range of Geant4-DNA for proton transport in liquid water

Wednesday 24 April 2019 17:20 (20 minutes)

Proton beams used in radiotherapy treatments can reach energies up to 250 MeV for deep-seated tumours. However, the existing cross section models included in Geant4-DNA [1,2] cover up to 100 MeV only. The goal of this work is to extend the current applicability range of Geant4-DNA for proton transport in liquid water up to, at least, 250 MeV.

Due to the energy range considered, the relativistic quantum mechanics theory is used following the work done by F. Salvat [3] in order to obtain an expression of the doubly-differential cross section (DDCS) with respect to the energy transferred, W, and recoil energy, Q. The latter is defined as the kinetic energy of a free electron with momentum equal to the momentum transfer. Considering the interaction in first order perturbation and modelling the projectile as a free particle (plane wave), the so-called Relativistic Plane Wave Born Approximation (RPWBA), the contributions of the projectile and the target to the DDCS appears separately. This approximation is only valid for incident energies of the projectile much larger than the typical ionization and excitation energies of the media. In the case of liquid water molecules, the largest value is around 500 eV. Under these conditions, the DDCS becomes proportional to the projectile charge and inversely proportional to its squared velocity. As for the target, its contribution is represented bythe generalized oscillator strength (GOS). The difficulty in its numeric calculation is due to the complexity of electronic wave-functions of liquid water molecules: spherical symmetry is not fulfilled because of the non-central potential and, additionally, they are perturbed by the effect of the interaction between molecules in the condensed phase. Modelling of GOS is, then, necessary. We split the GOS model into two Q ranges, low-Q (distant interactions) and large-Q (close interactions). For distant interactions, the GOS is modelled using semi-empirical optical dielectric functions of liquid water obtained in [4]. In the case of close interactions, the GOS is modelled as if the electrons of the liquid water were free and at rest. This way of GOS modelling allow us to obtain the contribution to the DDCS of each shell of the liquid water separately.

Once DDCS have been obtained, it is possible to calculate other magnitudes, such as cross sections or the stopping power. In the absence of cross section experimental data for the energy range of interest in this work, we have compared our calculation of the mass stopping power with the PSTAR tabulated values, founding a notable agreement from 1 MeV to 10 GeV.

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Session Classification: Medical applications

Track Classification: Medical applications