Title: Calculation of chemical species yields in liquid water after high energy electron irradiation up to 10 MeV using Geant4-DNA

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Background: Accurate simulation of water radiolysis by energetic electrons represents an important step towards developing mechanistic dose-response models of radiation action at the cellular level. The aim of this study is to calculate the chemical species yields (or G-values) of high-energy incident electrons over a broad energy range (50 keV-10 MeV). In this context, the Geant4-DNA [1] Monte Carlo toolkit provides the necessary physics and chemistry models to study electron track structures and their chemical evolution in liquid water medium.

Material and Methods: The Geant4-DNA option4 physics constructor was recently improved and extended up to 10 MeV for electron excitation and ionization processes [2]. Using this extended version and Geant4-DNA Chem6 example, we calculated the chemical yields of hydroxyl radical ($^{\bullet}OH$), hydrogen peroxide (H_2O_2) and solvated electron (e^-_{aq}) from 1 ps until 1 µs after irradiation. The chemical stage was simulated based on the IRT method [3]. This is the first study that demonstrates the application of Geant4-DNA physics and chemistry models in the energy regime of electron beam radiotherapy.

Preliminary results: Chemical yields (G values) of the three species were calculated for several electron energies between 50 keV and 10 MeV. A limited difference in G values at 1 ps was observed, after which the variation increased up until 1 µs. Figure 1 shows that G values at 1 µs have a direct dependence on the incident energies.

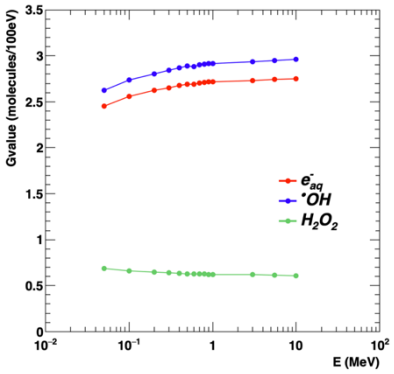

Figure 1: G values of e^-_{aq}, $^{\bullet}OH$ and H_2O_2 at 1µs as a function of incident electron energy.

[1] S. Incerti*et al.*Int J Model SimulSci Comput 1 (2010) 157-178
[2] I. Kyriakou*et al.* Front. Phys. 9 (2022) 711317
[3] J. Ramos-Mendez et al. Med. Phys. 47 (2020) 5919-5930