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Ionising radiation effects on DNA using Geant4-DNA Monte Carlo simulations

Monte Carlo track structure codes usually simulate particle tracks in liquid water since it makes up to 70% of living cells. Since DNA is considered the most radio sensitive target within eukaryotic cells simulating particle tracks within the DNA molecule is of high interest [1]. We implemented physics models of electrons in the 4 DNA bases as well as the sugar and the phosphate group on DNA as an extension of the Geant4-DNA option 6 that already exists for liquid water [2]. Elastic scattering, excitation and ionisation of electrons were implemented as physics models in Geant4-DNA according to the three interaction cross sections in the 6 different materials [3-4]. The models track electrons over the energy range of 11 eV –1 MeV. The calculated cross sections were in good agreement with results from the literature. The implemented models were tested for range and stopping power calculation in the various materials. We found a good agreement with calculations done by others specially for high energies and some deviation at the low energy that may be attributed to the difference in calculation models. A clear difference can be seen between liquid water calculations and the DNA material calculations which emphasizes the importance of simulations in the molecule itself. In addition, we are expanding the DNA geometry library of the "molecularDNA"example of Geant4-DNA dedicated to estimate the radio-induced damage in DNA models [5]. For this purpose, pBR322 plasmid DNA geometry was implemented in the example. A total of 104 circular plasmids are placed with random 3D orientations within a 6.5 micron radius sphere to reproduce the experimental density. The material used is liquid water for all structures and the whole geometry is irradiated with a monoenergetic electron beam. Preliminary results for the irradiation of dry plasmids with 5.5 MeV electrons, where only direct effects are considered, are a SSB yield of 0.35+/-0.02Gy-1Mbp-1for the simulation compared to 0.42+/-0.07 Gy-1Mbp-1 for the experiment [6]. Indirect damage simulations are ongoing and experimental validation for SSB and DSB yields is under investigation.

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Classification de Session: Pôle Effets des Irradiations sur le Vivant