INVESTIGATION OF GEANT4-DNA CHEMICAL YIELDS AND COMPARISON WITH RITRACKS AND EXPERIMENTAL OBSERVATIONS

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Introduction: Indirect damage due to reactive oxygen species (ROS) is responsible for a large proportion of the biological effect of radiation [1]. Additionally, there are effects such as in gold nanoparticle radiosensitisation for a proton beam which a) cannot be readily explained by traditional simulations of direct damage to DNA [2] and b) indicate a significant contribution from ROS [3]. Simulations of ROS production and interactions such as the newly added DNA chemistry models [4, 5] in Geant4 [6] are essential to simulating these effects. It is important when using models to understand the uncertainty of the simulation. However, this is difficult for chemistry models due to their spatio-temporal complexity and a large number of variables including the initial yields of ROS, and their dispersion, reaction and dissociation rates. To investigate the uncertainties, ROS yields were compared between Geant4-DNA chemistry and RITRACKS [7, 8], and published experiments for radiation types with differing linear energy transfer.

Methods: Computational simulations of the yield G (molecules/100eV) for ROS were performed using Geant4-DNA chemistry and RITRACKS. To properly compare chemistry models the simulations must have as close to an identical configuration as possible. By default in Geant4 the primary particle is killed in yield calculations once it has lost a certain amount of kinetic energy while in RITRACKS primary and secondary particles are killed upon leaving a volume. As Geant4 is more easily modified the volume method was used for comparisons.

Results: Initial yields of primary ROS (eg the hydroxyl radical, Figure 1) at one picosecond after physical interactions are similar for Geant4 and Ritracks simulations. However at greater times, differences in yields become larger. This indicates different reaction rates between the simulations. This results in large differences in yields of secondary ROS (eg hydrogen peroxide, Figure 2). Differences in initial yields of seconday ROS is due to RITRACKS starting the tracking of chemical species earlier in the physico-chemical stage.

Conclusions: Comparison of chemical yields from different simulations allows a qualitative understanding of simulation uncertainties. Yields of primary ROS have smaller discrepency especially at early times in the chemical stage. Yields of secondary ROS are more uncertain due to differences in ROS reaction rates. Comparison with experimentally observed chemical yields offers potential for improving chemical models and a reduction in their uncertainty.

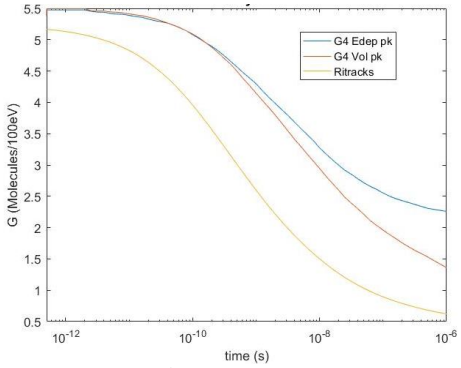

Figure 1. Plot of 1 MeV proton hydroxyl radical yields

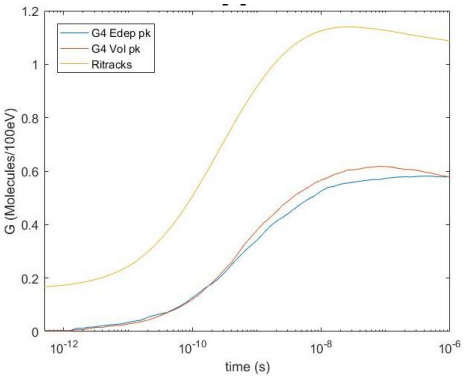

Figure 2. Plot of 1 MeV proton hydrogen peroxide yields

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