AbstractID: 3745 Title: A Monte Carlo model to simulate single and double strand breaks in DNA molecules

Purpose: One of the most confounding issues in the treatment of cancer is that two patients with the same diagnosis respond differently to the same treatment. The ultimate goal of this research effort is to better understand why this occurs. As a first step, the study presented here is performed to develop a system of computer codes to model the complex reactions between ionizing radiation and DNA.
Method and Materials: A mathematical atomistic model of a 167 base-pair B-DNA molecule was constructed using commercially available software packages. The probability of each possible fate of an •OH approaching to this 167 base-pair molecule was determined by implementing the "near-approach" DNA-radiation chemistry computational model described by Aydogan et al. (Radiat Res 157(1), 38-44, 2002) and compiled into an outcomes database. The secondary electron spectrum generated at depth in tissue by a Co-60 beam was modeled using the code MCNP 4.B. Two microdosimetry codes, OREC and RADLYS, originally developed at Oak Ridge National Laboratory, were adapted for this research. Attack sites were logged and single strand break (ssb) and double strand break (dsb) rates were calculated.
Results: At a dose of 100 Gy, the concentration scaled dsb per molecule was only 0.4 which is in good agreement with the dsb data which is 0.43 dsb/ molecule from the computational effort described in this report. **Conclusion:** A Monte Carlo calculation model has been shown to simulate single and double strand breaks using a novel computational approach presented authors previously that reduces the computation time and eliminates unnecessary repetition of the computationally expensive near chemistry simulation in DNA damage. Experimental comparison of the single and double strand break yields calculated in this study have shown the accuracy of the DNA damage simulation model presented.