Abstract

A radiation chemistry code based on the Green's function of the diffusion equation

Ianik Plante[1], Honglu Wu[2]

[1]USRA/Division of Space Life Sciences, NASA Johnson Space Center, Mail Code SK, Houston, TX 77058
[2]Human Adaptation and Countermeasures Division, NASA Johnson Space Center, Mail Code SK, Houston, TX 77058

Stochastic radiation track structure codes are of great interest for space radiation studies and hadron therapy in medicine [1]. These codes are used for a many purposes, notably for microdosimetry and DNA damage studies [2]. In the last two decades, they were also used with the Independent Reaction Times (IRT) method in the simulation of chemical reactions, to calculate the yield of various radiolytic species produced during the radiolysis of water and in chemical dosimeters [3]. Recently, we have developed a Green's function based code to simulate reversible chemical reactions with an intermediate state, which yielded results in excellent agreement with those obtained by using the IRT method [4]. This code was also used to simulate and the interaction of particles with membrane receptors [5, 6]. We are in the process of including this program for use with the Monte-Carlo track structure code Relativistic Ion Tracks (RITRACKS). This recent addition should greatly expand the capabilities of RITRACKS, notably to simulate DNA damage by both the direct and indirect effect.

References:

[1] Nikjoo, H. et al. *Radiat. Meas.* **41**, 1052-1074 (2006).
[2] Friedland, W. et al. *Radiat. Prot. Dosim.* **143**, 542-548 (2011).
[3] Autsavapromporn, N. et al. *Can. J. Chem.* **85**, 214-229 (2007).
[4] Plante, I. et al. *J. Comput. Phys.* **242**, 531-543 (2011).
[5] Plante, I. et al. *Phys. Rev. E* **84**, 051920 (2011).
[6] Plante, I. et al. *Comput. Phys. Comm.*, in press.