A radiation chemistry code based on the Green's Functions of the Diffusion Equation

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Abstract

Ionizing radiation produces several radiolytic species such as $^{\cdot}OH$, e^{-}_{aq}, and $H^{\cdot}$ when interacting with biological matter. Following their creation, radiolytic species diffuse and chemically react with biological molecules such as DNA. Despite years of research, many questions on the DNA damage by ionizing radiation remains, notably on the indirect effect, i.e. the damage resulting from the reactions of the radiolytic species with DNA. To simulate DNA damage by ionizing radiation, we are developing a step-by-step radiation chemistry code that is based on the Green's functions of the diffusion equation (GFDE), which is able to follow the trajectories of all particles and their reactions with time. In the recent years, simulations based on the GFDE have been used extensively in biochemistry [1], notably to simulate biochemical networks in time and space [2] and are often used as the "gold standard" to validate diffusion-reaction theories. The exact GFDE for partially diffusion-controlled reactions is difficult to use because of its complex form. Therefore, the radial Green's function, which is much simpler, is often used [3]. Hence, much effort has been devoted to the sampling of the radial Green's functions, for which we have developed a sampling algorithm [4]. This algorithm only yields the inter-particle distance vector length after a time step; the sampling of the deviation angle of the inter-particle vector is not taken into consideration. In this work, we show that the radial distribution is predicted by the exact radial Green's function. We also use a technique developed by Clifford et al. [5] to generate the inter-particle vector deviation angles, knowing the inter-particle vector length before and after a time step. The results are compared with those predicted by the exact GFDE and by the analytical angular functions for free diffusion. This first step in the creation of the radiation chemistry code should help the understanding of the contribution of the indirect effect in the formation of DNA damage and double-strand breaks.

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