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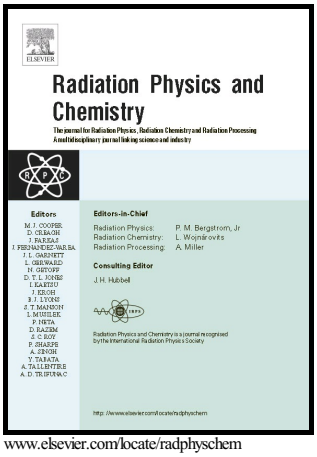

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Considerations for the independent reaction times and step-by-step methods for radiation chemistry simulations

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Abstract

Ionizing radiation interacts with the water molecules of the tissues mostly by ionizations and excitations, which result in the formation of the radiation track structure and the creation of radiolytic species such as $H^{\bullet}$, $^{\bullet}OH$, H_2, H_2O_2, and e^-_{aq}. After their creation, these species diffuse and may chemically react with the neighboring species and with the molecules of the medium. Therefore radiation chemistry is of great importance in radiation biology. As the chemical species are not distributed homogeneously, the use of conventional models of homogeneous reactions cannot completely describe the reaction kinetics of the particles. Actually, many simulations of radiation chemistry are done using the Independent Reaction Time (IRT) method, which is a very fast technique to calculate radiochemical yields but do not calculate the positions of the radiolytic species as a function of time. Step-by-step (SBS) methods, which are able to provide such information, have been used only sparsely because these are time-consuming in terms of calculation. Recent improvements in computer performance now allow the regular use of the SBS method in radiation chemistry. The SBS and IRT methods are both based on the Green's functions of the diffusion equation (GFDE). In this paper, several sampling algorithms of the GFDE and for the IRT method are presented. We show that the IRT method is exact for 2-particles systems for diffusion and partially diffusion-controlled reactions between non-interacting particles. We also show that the results obtained with the SBS simulation method with periodic boundary conditions are in agreement with the predictions by classical reaction kinetics theory, which is an important step towards using this method for modelling of biochemical networks and metabolic pathways involved in oxidative stress. Finally, the first simulation results obtained with the code RITRACKS (Relativistic Ion Tracks) are presented.