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TRAX-CHEM: a pre-chemical and chemical stage extension of the particle track structure code TRAX in water targets

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Abstract

The production, diffusion, and interaction of particle beam induced water-derived radicals is studied with the a pre-chemical and chemical module of the Monte Carlo particle track structure code TRAX, based on a step by step approach. After a description of the model implemented, the chemical evolution of the most important products of water radiolysis is studied for electron, proton, helium, and carbon ion radiation at different energies. The validity of the model is verified by comparing the calculated time and LET dependent yield with experimental data from literature and other simulation approaches.

Keywords: Water Radiolysis, Ion Radiation, Monte Carlo Simulations, Track Structure

1. Introduction

The indirect effect of radiation plays a very important role in the mechanism of radiation impact on biological systems and many dosimetric techniques are based on the detection of chemical reactions with radiation induced free radicals. In particular, the reaction of chemical species generated during water radiolysis results to be especially important, as they are responsible for a large portion of the radiation-induced biological damage. For charged particle radiation, however, few experimental data are available

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