Contribution ID : **46** Type : **not specified**

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

The indirect effect of radiation plays a very important role on the radiation effect on biological systems. The interaction of chemical species generated during water radiolysis, among themselves and with the target material, results to be especially relevant as they are responsible for a large portion of the radiation-induced biological damage. However the nanoscopic processes and mechanisms underlying the radicals diffusion and reaction along a particle track are still not completely known. In this context, the development of models and tools able to describe the chemical track evolution will allow not only to better investigate the indirect effect of radiation damage, but also to access problems where the chemical pathway seems unavoidable, namely nanoparticles sensitisation effect, the impact of the target oxygenation level on the tissue radiosensitivity and the possibility of investigating the role of radical scavengers on the chemical kinetics along an ion track.
Monte Carlo track structure codes are particularly suitable for studying the microscopic processes involved in the radiation damage thanks to their capability to handle the stochastic nature of radiation interaction with the target material. In this poster, the new implementation of the pre-chemical and chemical module of the Monte Carlo particle track structure code TRAX will be presented. Thanks to this extension the code is now able to describe with a step by step approach the production, diffusion and reaction of particle beam induced water-derived radicals. After a description of the implemented model, the chemical evolution of the most important products of water radiolysis, e^-_{aq}, $OH\cdot$, $H\cdot$, H_3O^+, H_2, OH^- and H_2O_2 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.

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