

Current development status of simulation code for physical and chemical processes in PHITS/PHITS における物理・化学過程のシミュレーションコードの開発状況

Radiation-induced biological effects such as cell death and mutation are believed to be attributed to initial DNA damage induction by energy deposition (physical processes) and reactions of chemical products to DNA (chemical processes). The mechanisms of DNA damage induction remain unclear. To make clear the mechanisms, the development of the simulation codes for physical and chemical processes is of great importance. In this presentation, we introduce the current development status of the simulation codes for physical and chemical processes in Particle and Heavy Ion Transport code System (PHITS) [1]. The physical processes of radiation in the human body can be simulated using track-structure modes in PHITS, i.e., PHITS-ETS and PHITS-KURBUC modes [2]. These track-structure modes consider each atomic interaction (such as elastic scattering, ionization, electronic excitation, dissociative electron attachment, vibrational excitation, photon excitation, rotational excitation, electron capture, and electron loss). Meanwhile, to simulate the physicochemical and chemical processes, we recently developed the PHITS-Chem mode [3]. The PHITS-Chem mode allows the calculation of the G values of 16 products (e.g., $\cdot\text{OH}$, e_{aq}^- , H_2 , and H_2O_2) and 35 chemical reactions as a function of time after irradiation (> 1 ps). Through this presentation, we present the features of PHITS-ETS, PHITS-KURBUC, and PHITS-Chem, and discuss the application of these codes to biological research.

References

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