

From Hadrons to Therapy: Fundamental Physics Driving New Medical Advances

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Track structure simulations in nano sized geometries

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Monte Carlo (MC) radiation transport codes for charged particles, including electrons, protons, light and heavy ions, provide detailed information about interaction types, spatial and temporal distributions of energy depositions, as well as radical species produced in the early physical and chemical states of radiation action with matter. This information allows to investigate the biological response to radiation and to determine the initial patterns of radiation damage in biological systems. MC codes depend on reliable interaction cross sections and transport models to produce viable results. General purpose codes use available cross section data bases and can simulate radiation transport in a wide variety of materials, while track structure codes are typically limited to a few materials like (liquid) water or cell constituents like DNA bases and density scaling is used to simulate other materials.

Radiation transport models include main basic assumptions: (a) all events are independent, (b) radiation equilibrium is observed, and (c) infinite and 3-dimensional transport in bulk media. If a particle passes through an interface, for example from one area of interest to another, the transport is stopped at the border, and a new event randomly selected in the new area. These assumptions work well if the dimensions of the areas of interest are sufficiently large compared to the mean free path, the average distance between two interactions. The Penelope code for example suggests that there should be at least 10 interactions within an area of interest to achieve radiation equilibrium. However, this situation changes when considering nano geometries, like nano particles. In this case, the mean free path is comparable to the geometry size. Transport model artefacts may be observed instead of realistic simulation results.

This communication investigates these basic assumptions and analyzes track structure simulations performed with the PARTRAC code for different geometries, from micrometer down to nanometer sizes. It is also known that cross section models change when going from infinite 3-dimensional transport (bulk) to 2-dimensional transport, i.e., through surfaces (see for example [1] and references therein). We also see differences in the experimentally obtained secondary electron emission spectra originating from bulk gold and gold nano particles; see for example contribution from Jeff Shinpaugh at this meeting.

REFERENCES

[1] M. Dingfelder and A. Travia, *Radiat. Prot. Dosim.* 166, 10-14 (2015).

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