

POTENTIAL IMPLEMENTATION OF NITROGEN, PROPANE AND DNA CROSS SECTIONS FOR ELECTRONS AND LIGHT IONS INTO GEANT4-DNA

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Introduction: Implementation of Geant4-DNA physics models are currently available only for use in liquid water. Simulations involving biological targets thus rely on the approximation of water (and its associated interaction cross sections) as a substitute for biological matter. While this approximation is considered sufficiently realistic down to the micrometric scale, inaccuracies may arise in track structure simulations involving detailed interaction of particles. Of particular concern is densely ionising radiation, such as ions with energy corresponding to their maximum stopping power or low-energy electrons below about 1 keV, as these particles deposit a large fraction of their energy within volumes of a few cubic micro- or nanometres.

The unsuitability of liquid water as a substitute extends to other applications in micro- and nanodosimetry, such the comparison of Geant4-DNA simulations with experiments. Microdosimeters often use tissue-equivalent gases comprising a mixture of propane, nitrogen and carbon dioxide, while nanodosimeters are usually operated with nitrogen or propane. Appropriate cross section data of these gases are therefore needed for accurate simulations.

Materials and methods: This work presents recommended cross section data sets of nitrogen and propane for electrons, protons and alpha particles to implement in Geant4-DNA [1-3]. These data sets comprise cross sections for ionisation and excitation as well as alpha particle charge-transfer and elastic scattering of electrons. Collaborative work is also in progress for implementing the cross sections of DNA constituents for electrons and light ions [4-6] in Geant4-DNA.

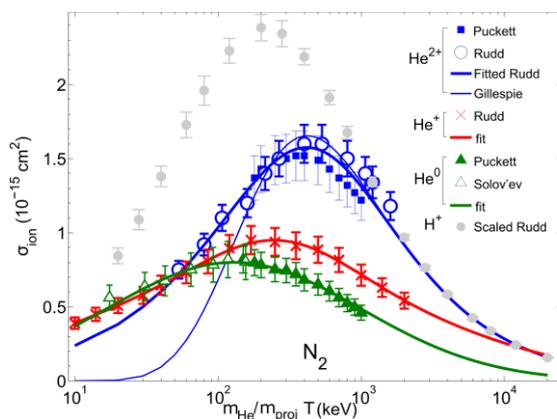


Figure 1. Measured and modelled cross sections σ_{ion} for ionisation of nitrogen by helium particles and protons [1].

Results: Cross section data of nitrogen and propane for light ions between 100 keV and 20 MeV as well as electrons down to the ionisation threshold have been evaluated and implemented into the PTB track structure code (PTra). Those implemented for ionisation of nitrogen by helium particles and protons can be seen in Figure 1. PTra simulations with all aforementioned data sets have been benchmarked against nanodosimetry experiments for protons and alpha particles [7]. Implementation of measured double-differential cross sections of nitrogen and propane, which describe the distribution of secondary electron emission angles, is also possible.

Conclusions: For Geant4-DNA simulations concerning experimental micro- and nanodosimetry, implementation of the proposed cross section data sets of nitrogen and propane could improve the accuracy of simulation results.

References

1. Ionization cross section data of nitrogen, methane, and propane for light ions and electrons and their suitability for use in track structure simulations (M. Bug et al.), *Phys. Rev. E* **88**, 043308 (2013).
2. Formation of ionization clusters in nanometric structures of propane-based tissue-equivalent gas or liquid water by electrons and α -particles (B. Grosswendt), *Radiat. Environ. Biophys.* **41**, 103–112 (2002).
3. The Formation of Ionisation Clusters by a Particles in 'Nanometric' Volumes of Nitrogen: Experiment and Calculation (B. Grosswendt and S. Pszozna), *Radiat. Prot. Dosimetry.* **99**, 331–335 (2002).
4. An electron-impact cross section data set (10 eV–1 keV) of DNA constituents based on consistent experimental data: A requisite for Monte Carlo simulations (M. Bug et al.), *Radiat. Phys. Chem.* **130**, 459–479 (2017).
5. Cross sections for ionization of tetrahydrofuran by protons at energies between 300 and 3000 keV (M. Wang et al.) *Phys. Rev. A* **93**, 052711 (2016).
6. Double differential cross sections for proton induced electron emission from molecular analogues of DNA constituents for energies in the Bragg peak region (B. Rudek) *J Chem Phys.* **145**, 104301 (2016).
7. Secondary ionisations in a wall-less ion-counting nanodosimeter: quantitative analysis and the effect on the comparison of measured and simulated track structure parameters (G. Hilgers et al.), *Eur. Phys. J. D.* **69**, 239–257 (2015).