

Microdosimetry and radiolytic species production in UHDR proton beam using GATE and Geant4-DNA

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ARRONAX cyclotron facility:

IBA Cyclone®70

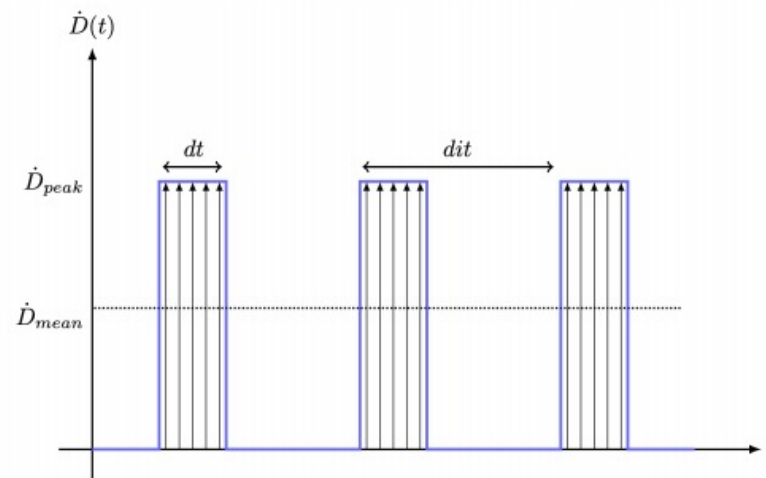
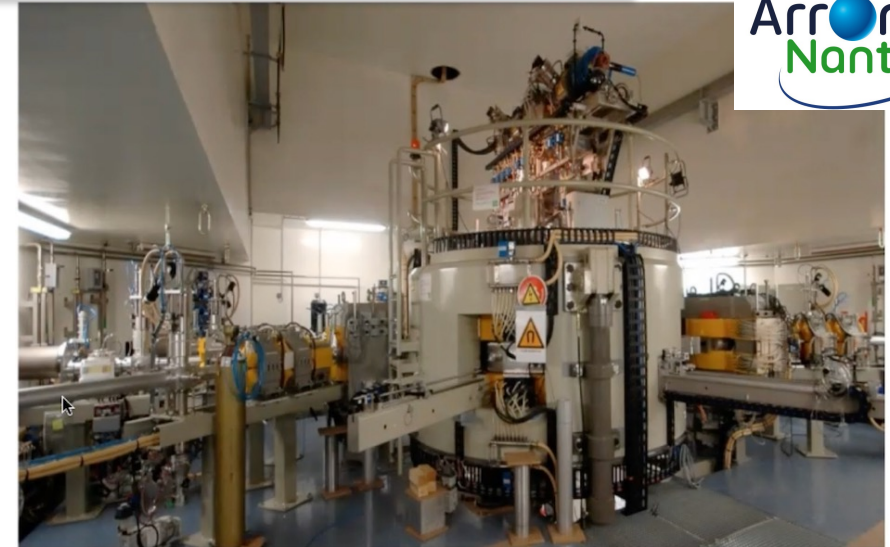
Protons, deuterium and alpha particles

Protons energy range: 30-70 MeV

(ranges in water: 8-38 mm)

Max dose rate > 7500 Gy/s

RT CONV ~ 0,3Gy/s



$dt = [0.67 - 10.67] \text{ ms}$

UHDR -> Single pulse

CONV -> Multiple pulses (100 Hz)

Radiobiology

Zebra fish irradiation

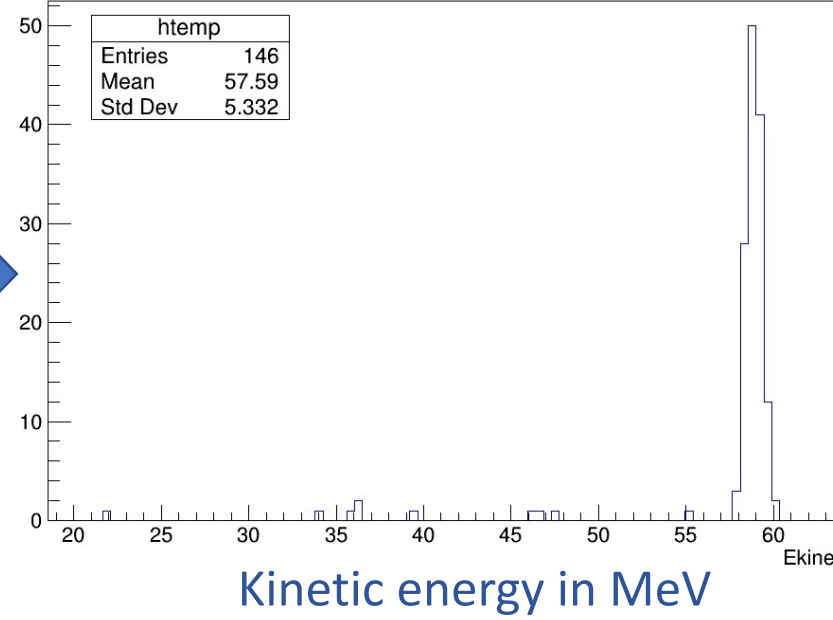
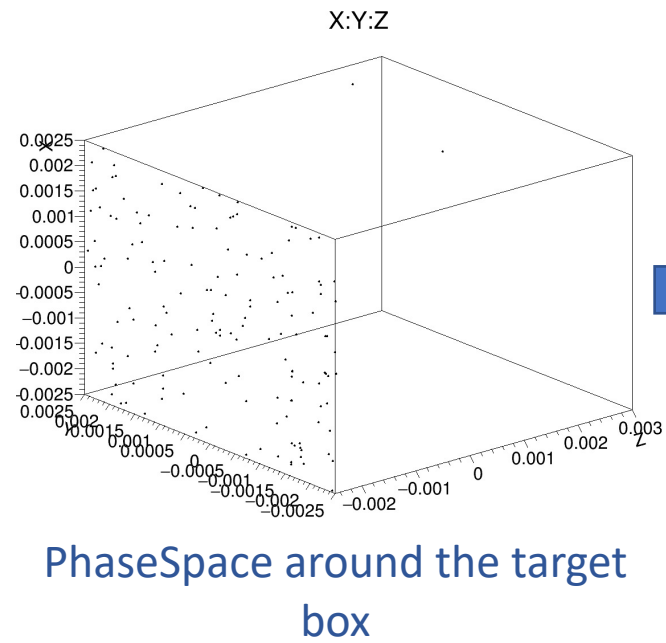
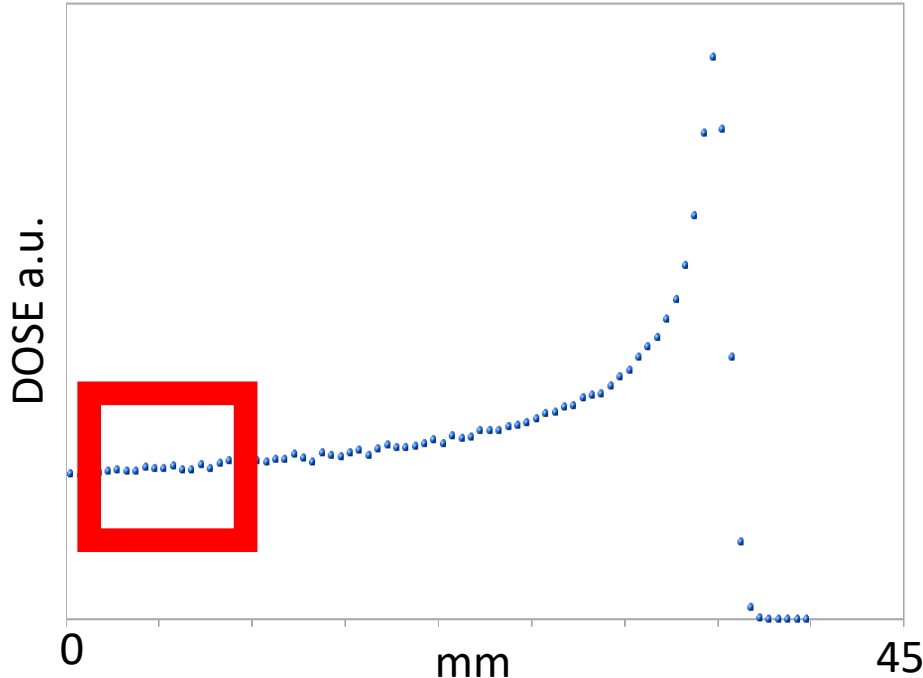
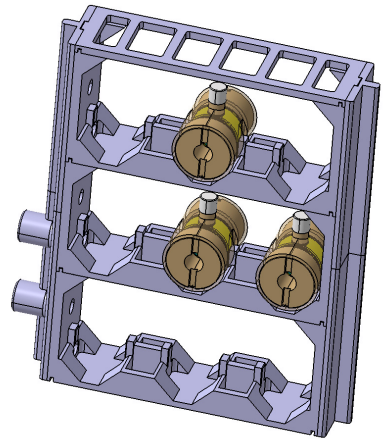
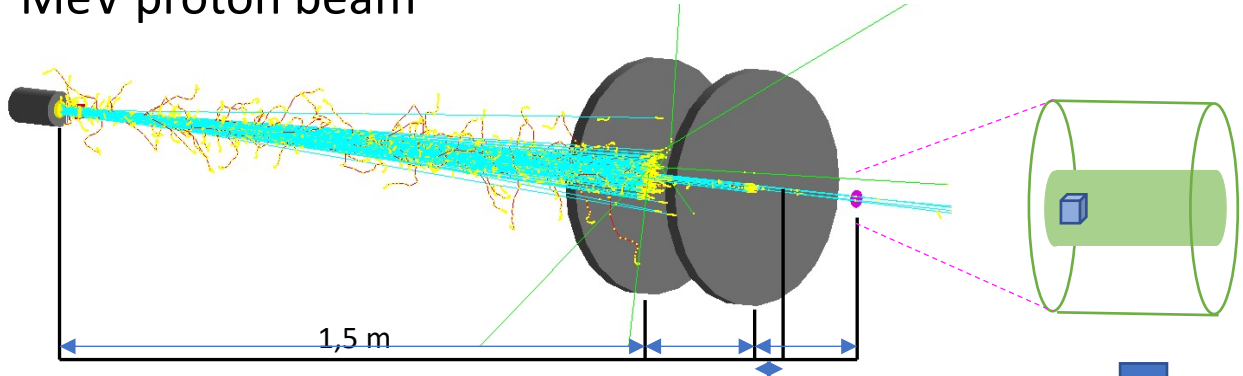
Human cells irradiation

Radiochemistry:

H₂O₂ measurements

Beam line simulation

67 MeV proton beam



CHEM6 example



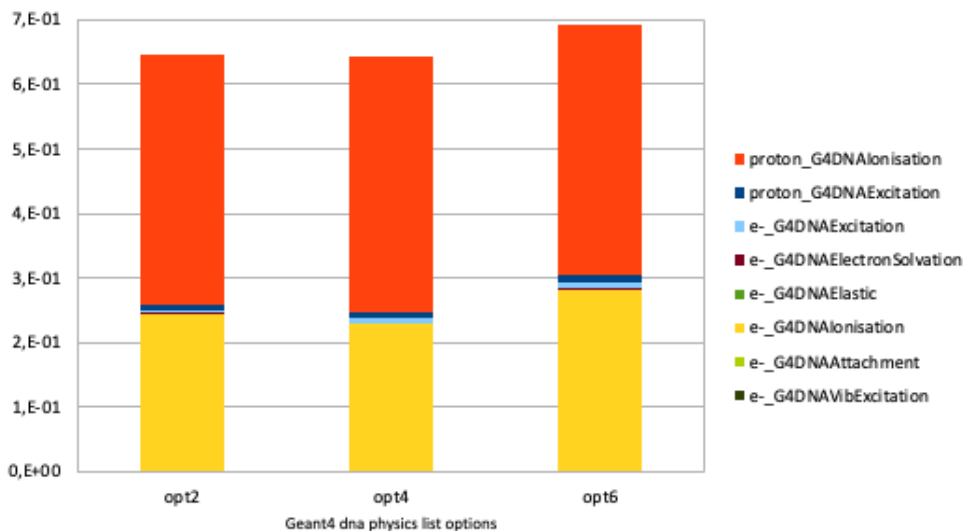
5 μm³ water cube

Conventional dose rate

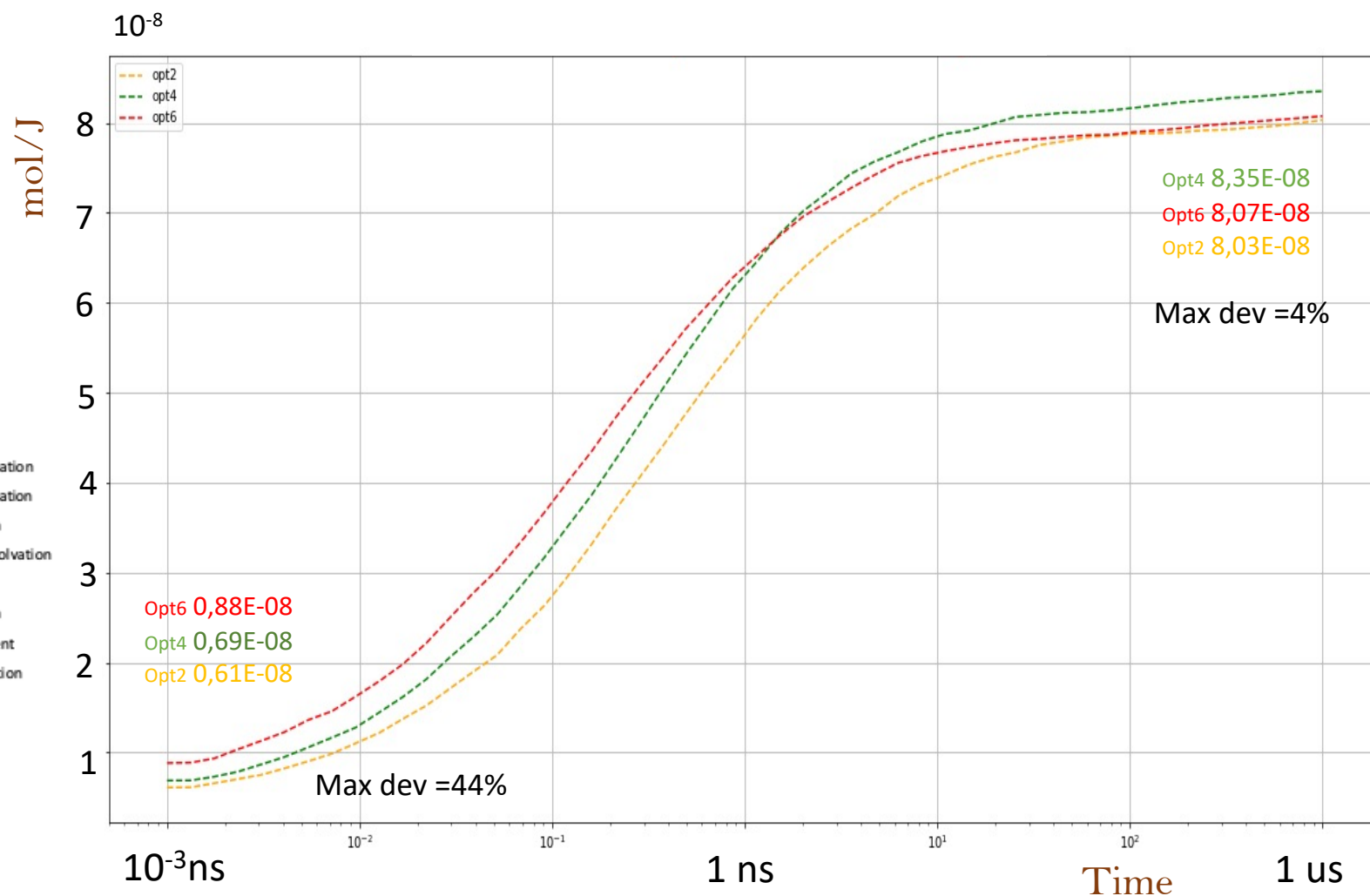
PhaseSpace around the cube.

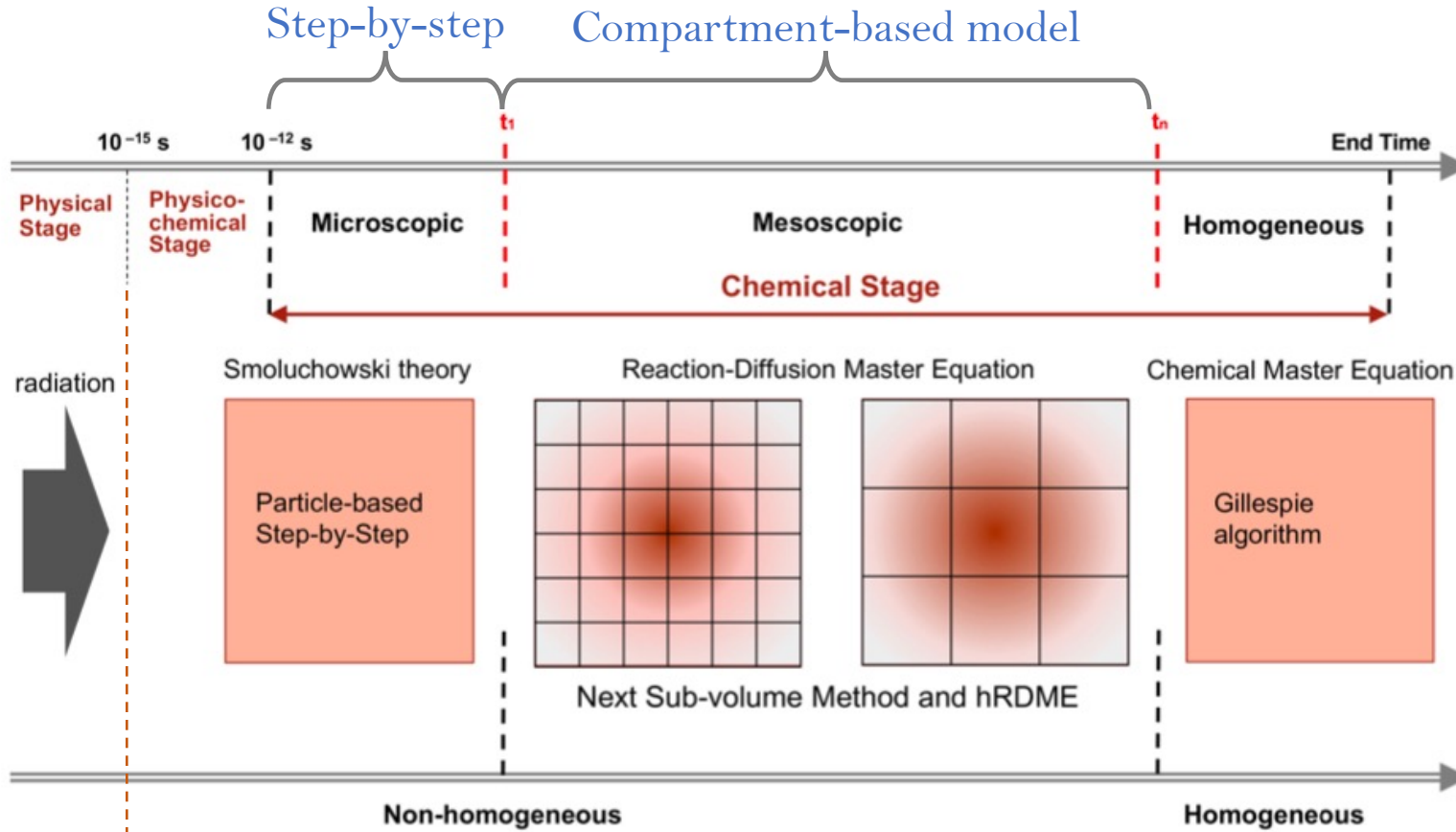
PhaseSpace source in HDF5 format.

Percentage contribution processes



H₂O₂ G values along time, using 3 physics lists





Chemical stage beyond the microsecond:

- Homogeneity within each voxel
- Diffusion of species between voxels
- Reaction between species within voxels
- Voxel size increases over time (heterogeneous -> homogeneous)

Simulated conditions:

- Aerated water radiolysis
- NO_2 scavenger
- Fricke dosimeter

Physical stage

What is a cutoff dose?

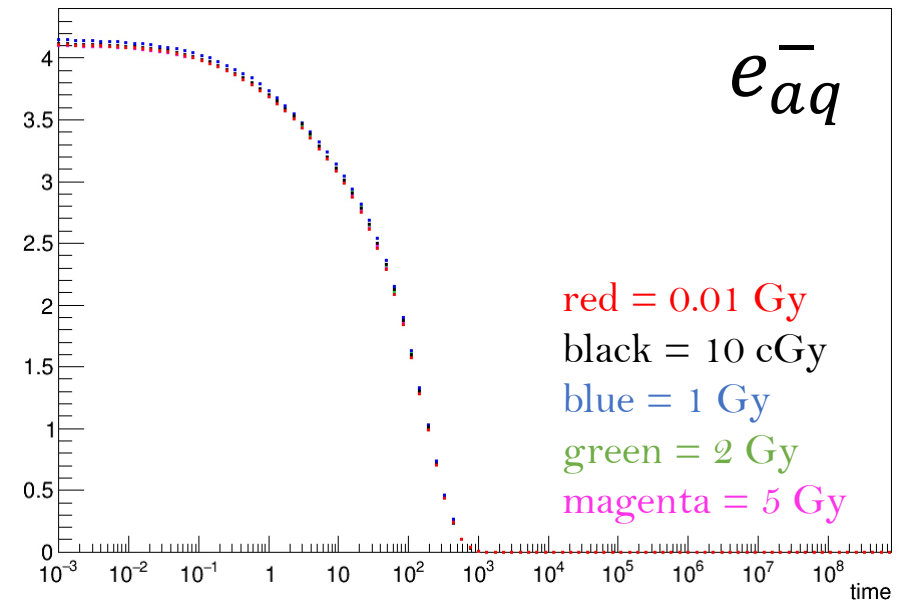
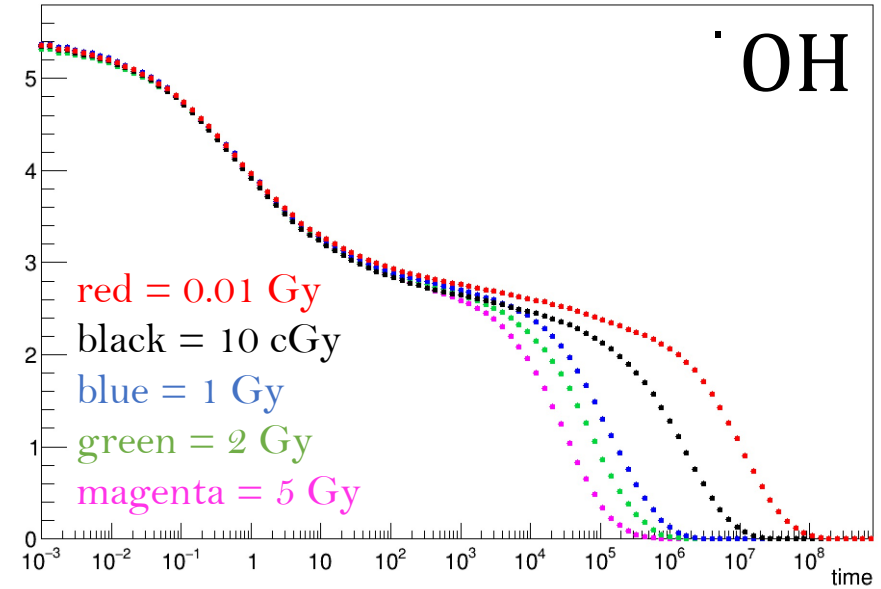
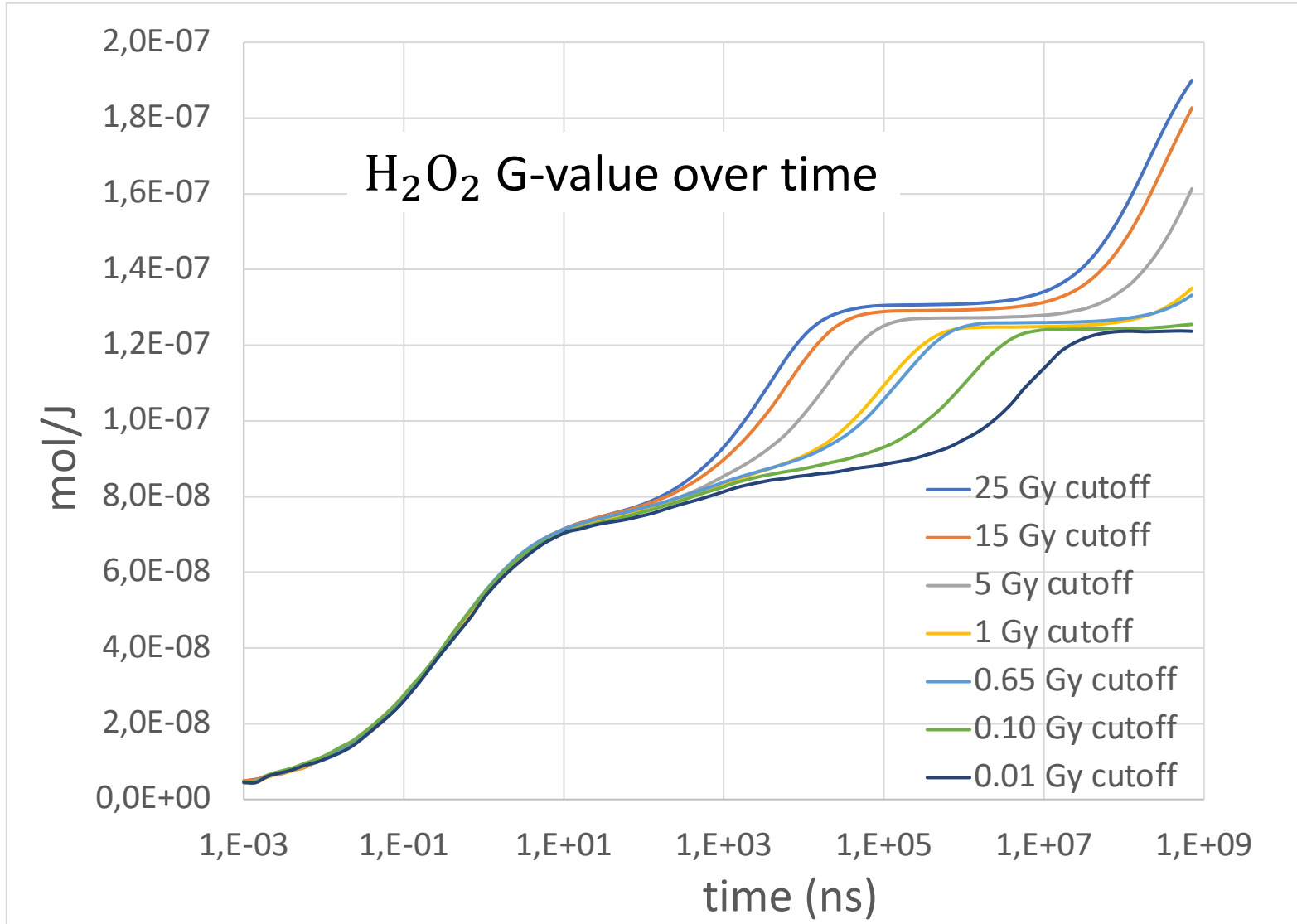
Protons are generated till a cutoff dose is reached

Tran, H.N.; Chappuis, F.; Incerti, S.; Bochud, F.; Desorgher, L.

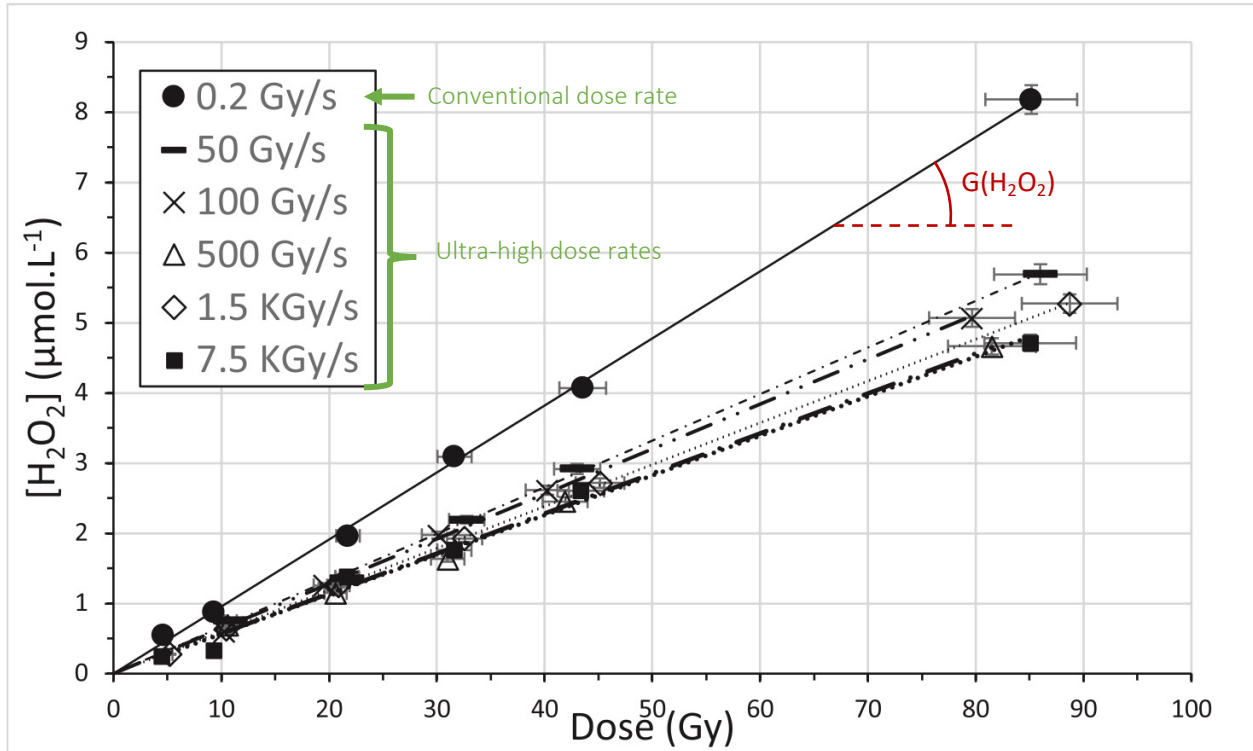
Geant4-DNA Modeling of Water Radiolysis beyond the Microsecond: An On-Lattice Stochastic Approach.

Int. J. Mol. Sci. **2021**, *22*, 6023. <https://doi.org/10.3390/ijms22116023>

57 MeV protons ➤ In aerated environment H_2O_2 production depends on the dose per pulse



Experimental measurements



Concentrations of H_2O_2 have been determined after irradiation about 15 minutes post irradiation.

The concentration of H_2O_2 was obtained indirectly by measurement of I_3^- absorbance using a spectrophotometer.

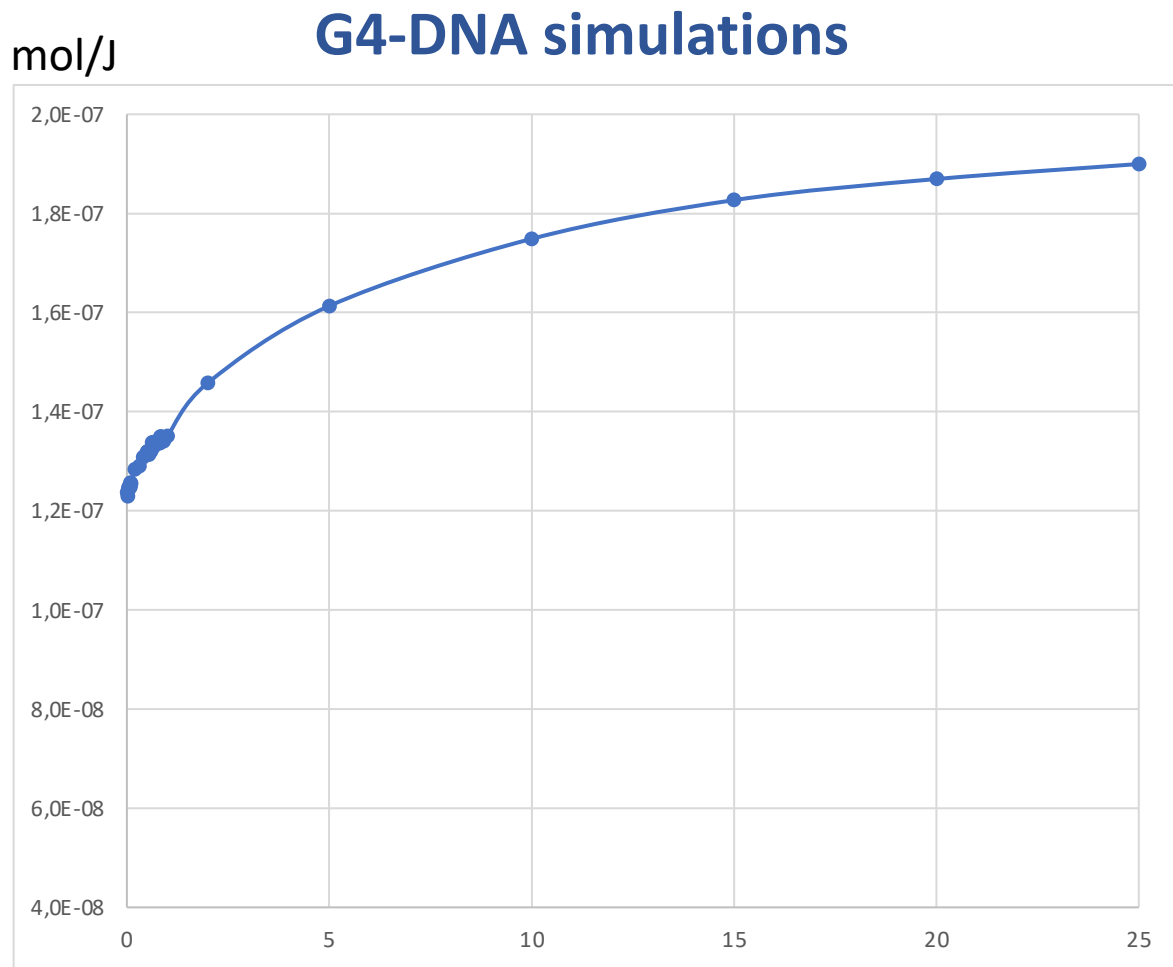
The radiolytic yield (G) is defined as the number of species formed or consumed per unit of deposit energy.

Blain, G. et al.

Proton Irradiation at Ultra-High Dose Rate vs. Conventional Dose Rate: Strong Impact on Hydrogen Peroxide Yield.

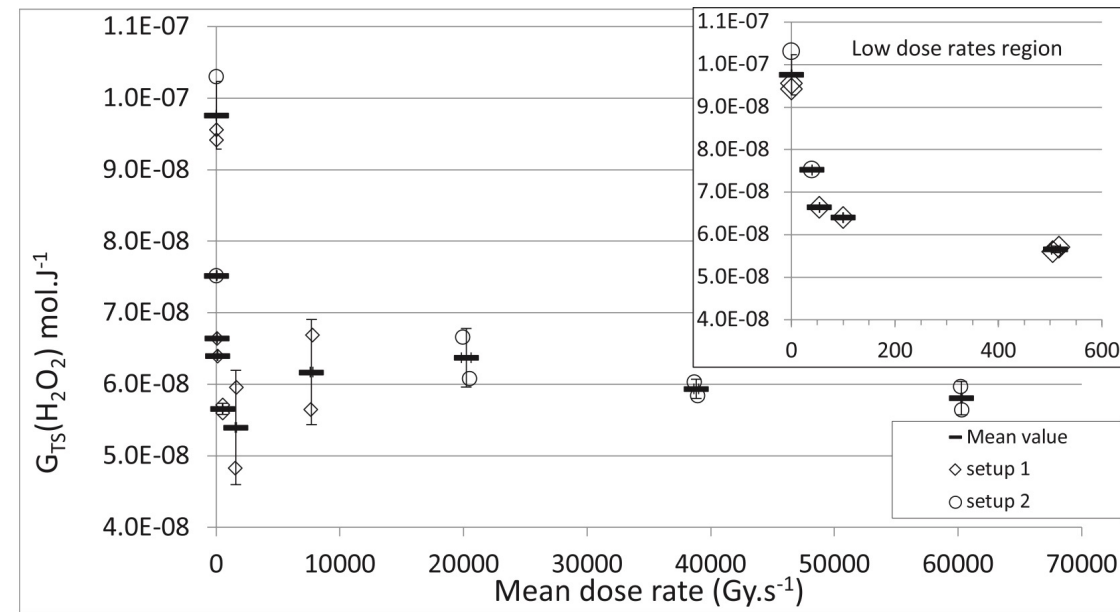
Radiation Research, **2022**, *198*, 318-324.

Simulations vs experimental measurements



Cutoff dose (toward higher dose rates)

Experience



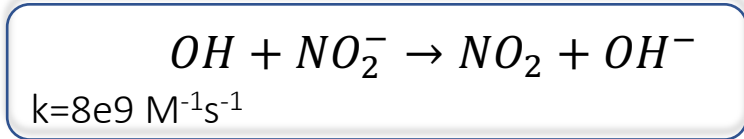
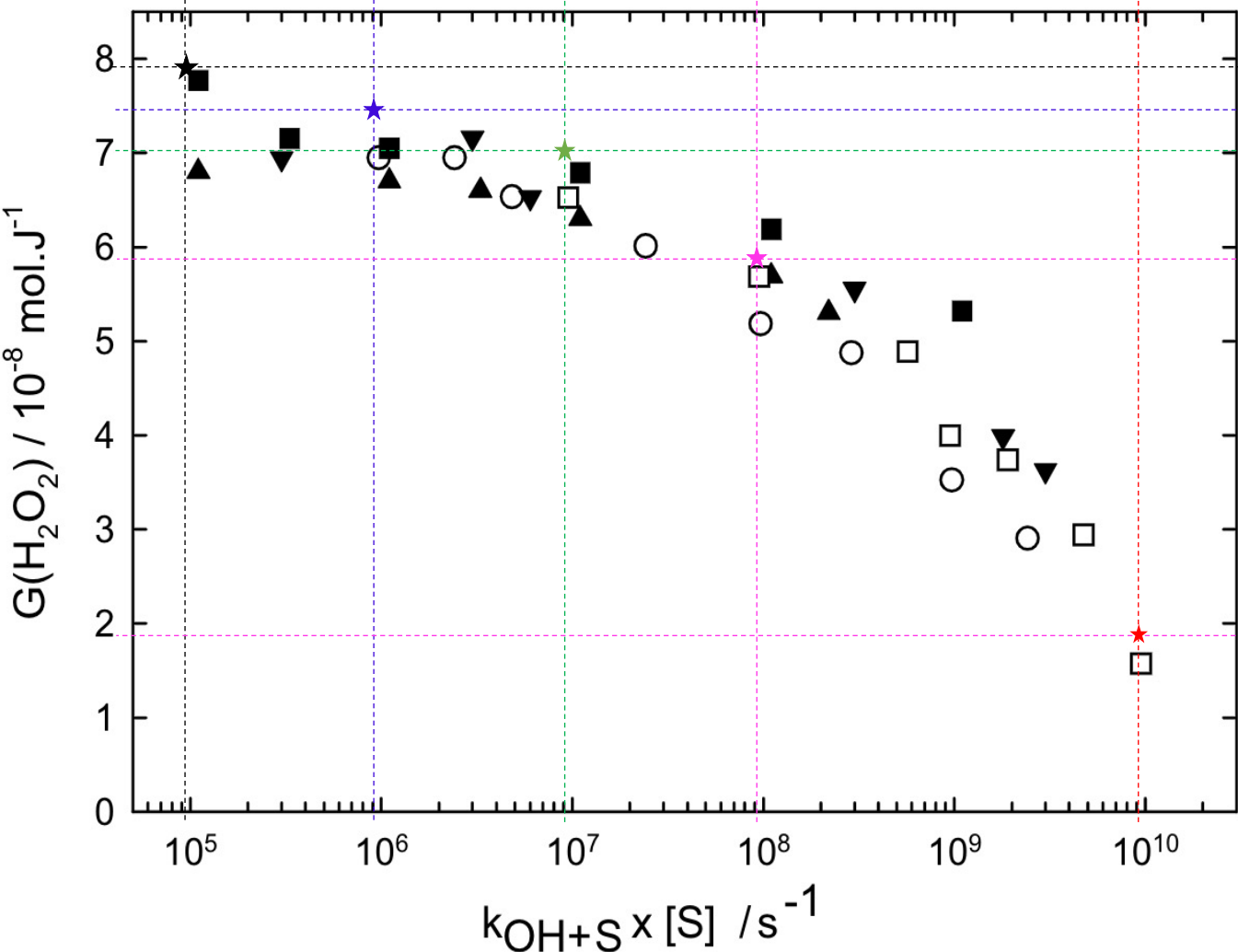
Blain, G. et al.

Proton Irradiation at Ultra-High Dose Rate vs. Conventional Dose Rate: Strong Impact on Hydrogen Peroxide Yield.
Radiation Research, 2022, 198, 318-324.

Hypothesis:

- pH variation
- Longer time

Hydrogen peroxide yields as a function of scavenging capacity of *OH radical for different solutes



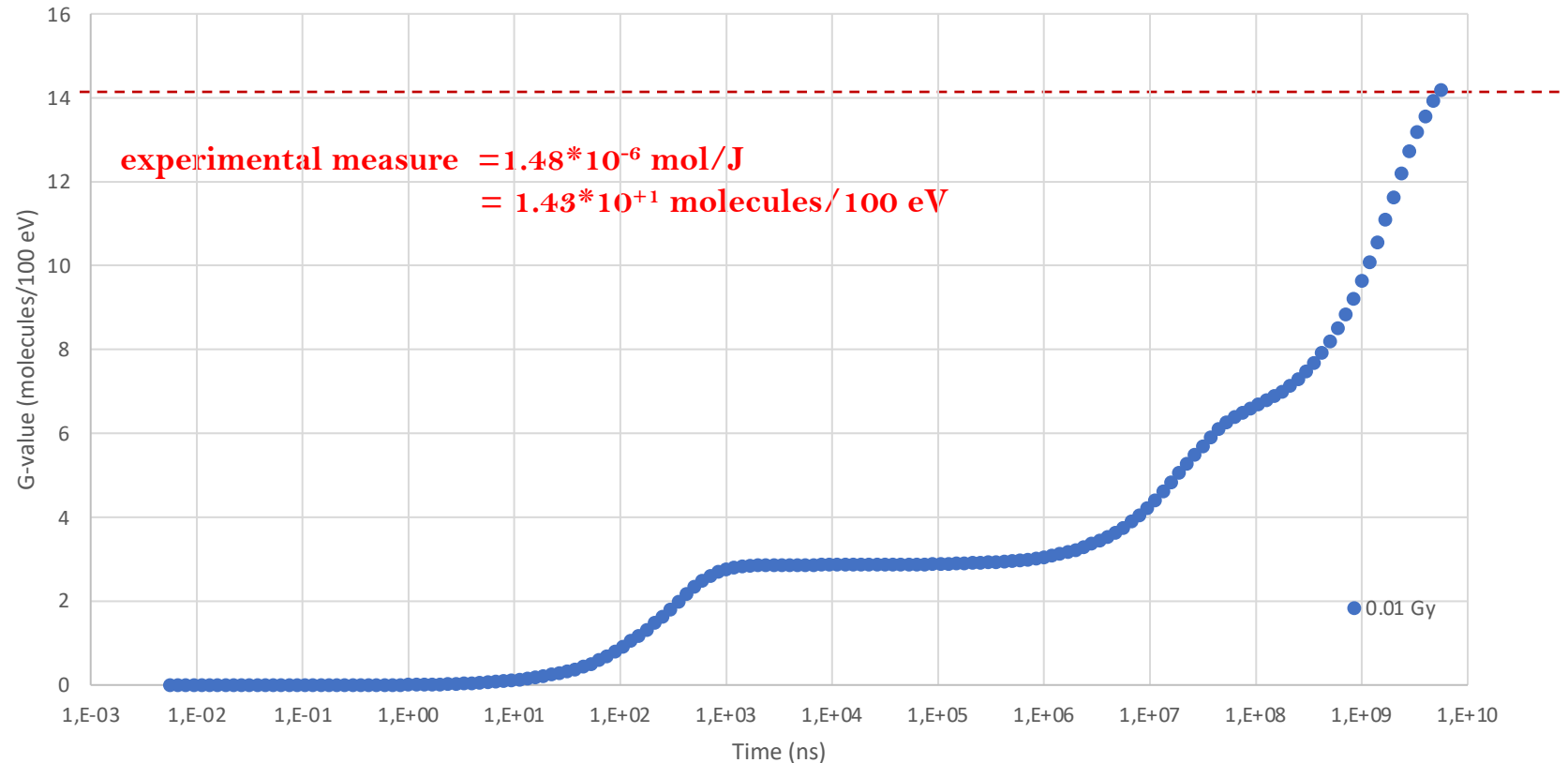
Proton 57 MeV

	0.0125 mM	0.125 mM	1.25 mM	12.5 mM	1.25 M
mol/J (10 ⁻⁸)	7.90	7.52	7.03	5.85	1.85

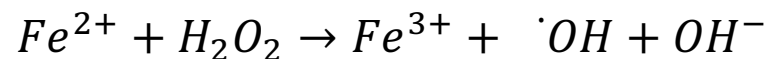
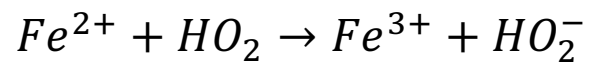
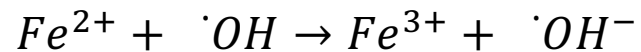
Hydrogen peroxide yields in water radiolysis by high-energy ion beams at constant LET
Wasselin-Trupin. Baldacchino. Bouffard. Hickel
Radiation Physics and Chemistry
Volume 65, Issue 1, August 2002, Pages 53-61

This dosimetry technique depends on the oxidation of ferrous ions (Fe^{2+}) to ferric ions (Fe^{3+}) by ionizing radiation.

The increased concentration of ferric ions is measured spectrophotometrically at 304 nm. The Fricke dosimeter is 96% water by weight; therefore, its dosimetric properties are very similar to those of water.



Added reactions



Added scavengers:

```
/chem/env/Scavenger O2 19 %
/chem/env/Scavenger Fepp 10 mM
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Fe^{3+} → yields are comparable with experimental measurements

Conclusion & perspectives

- Validated simulation of the beam line using GATE
- A new version of the Geant4-DNA chemistry module for water radiolysis simulation in UHDR conditions (with scavengers)
- H_2O_2 G-values \neq experimental measurements -> **WORK IN PROGRESS**
- NO_2 scavenging capacity validated with literature
- First results for Fricke dosimeter in conventional dose rate show good agreement with experimental measurements