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

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FLASHMOD

Proton FLASH irradiation at ARRONAX

ARRONAX cyclotron facility:

IBA Cyclone®70

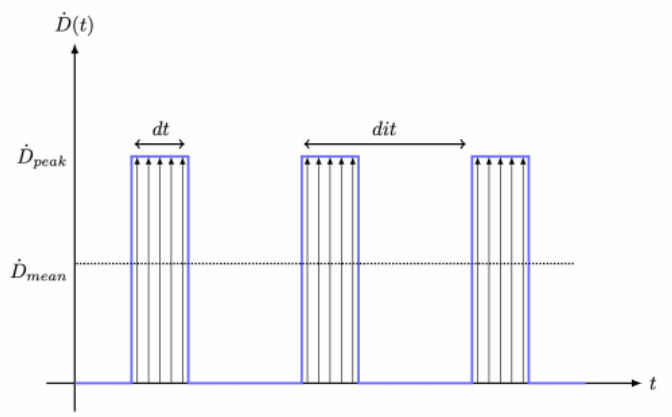
Protons, deuterium and alpha particles

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] ms

UHDR -> Single pulse

CONV -> Multiple pulses (100 Hz)

Radiobilogy

Zebra fish irradiation

Human cells irradiation

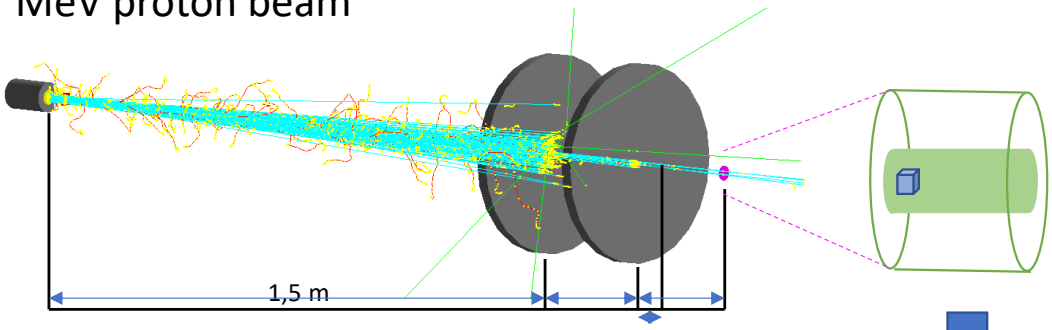
Radiochemistry:

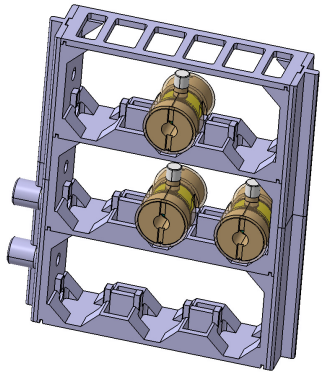
H_2O_2 measurements

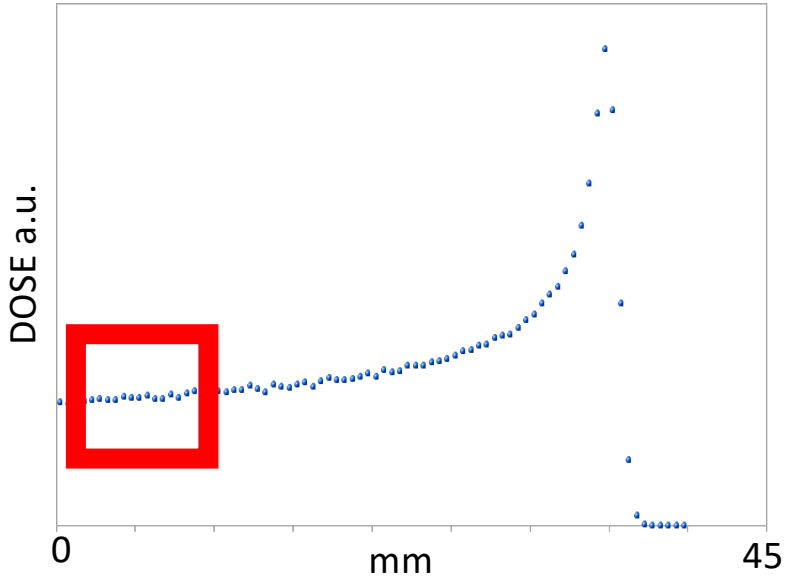
Beam line simulation

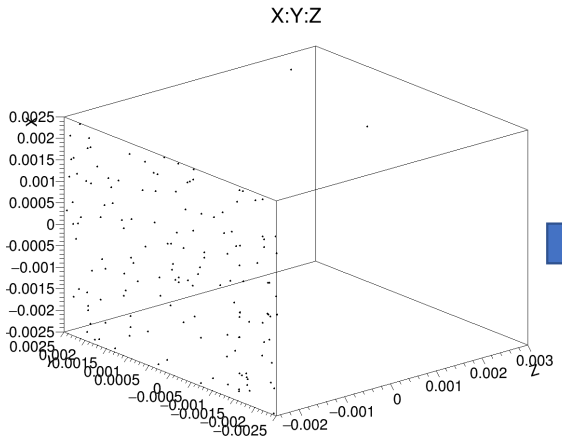
GATE v9.1

67 MeV proton beam

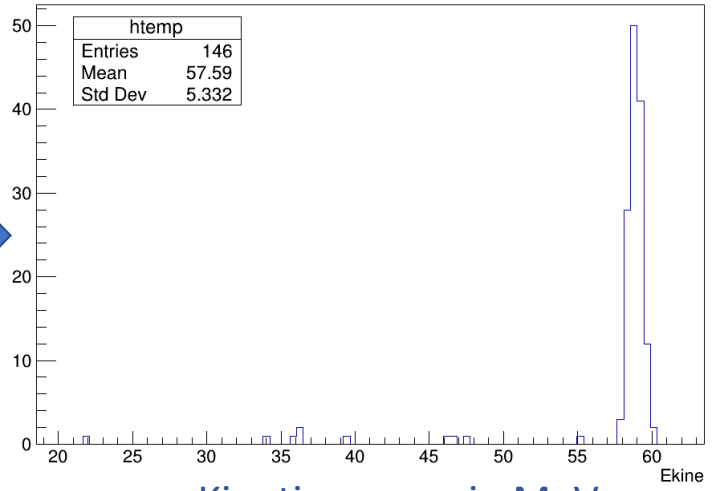








PhaseSpace around the target box

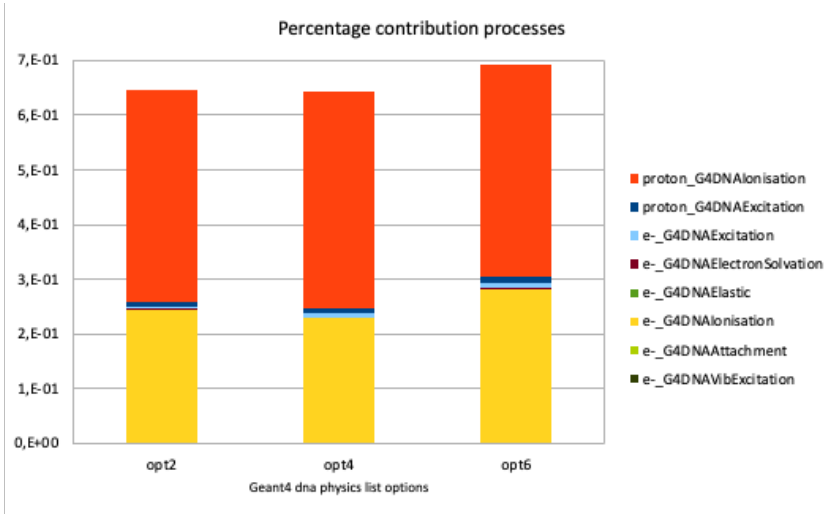


Kinetic energy in MeV

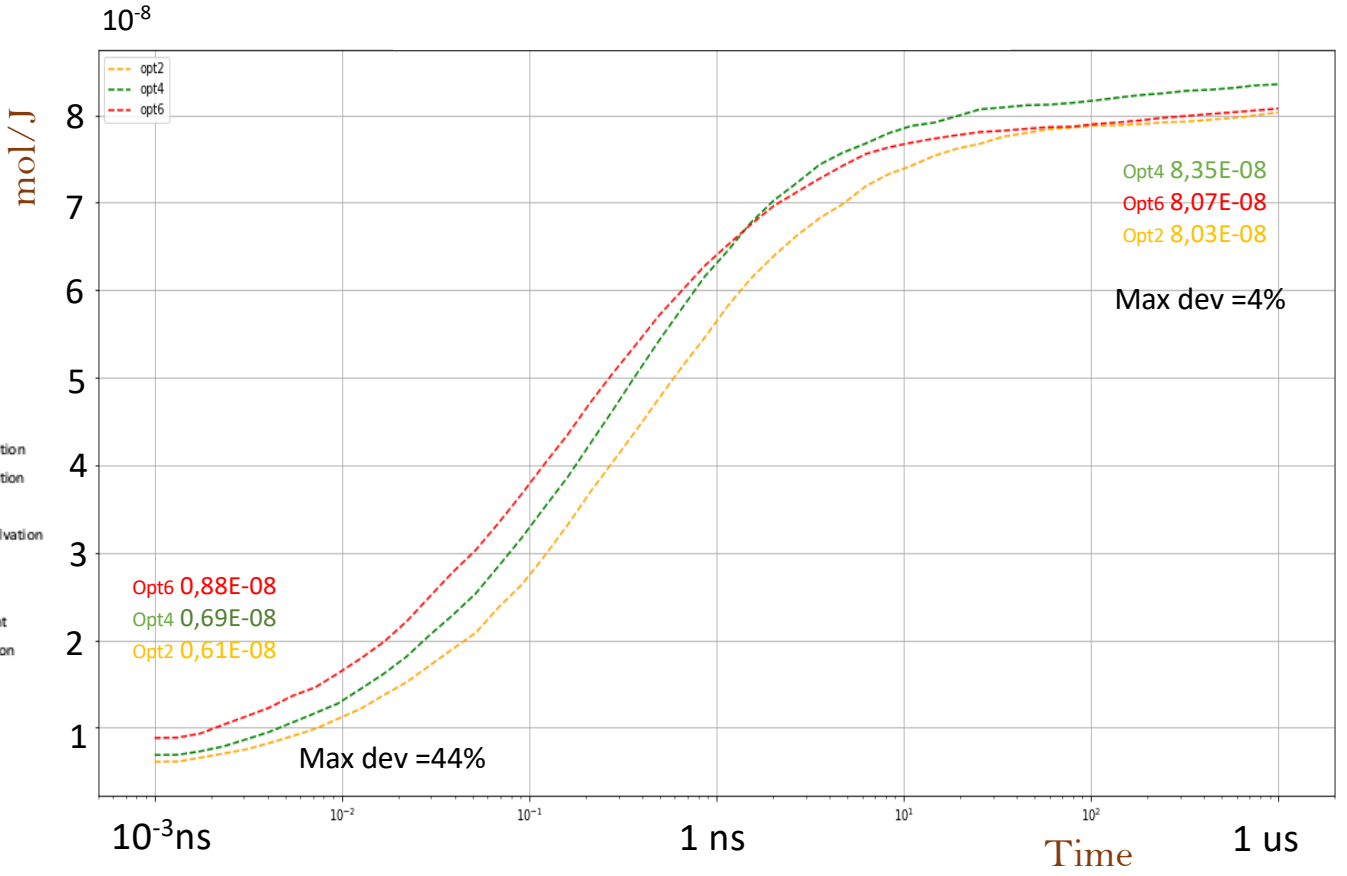
H_2O_2 G values - physicslists

CHEM6 example

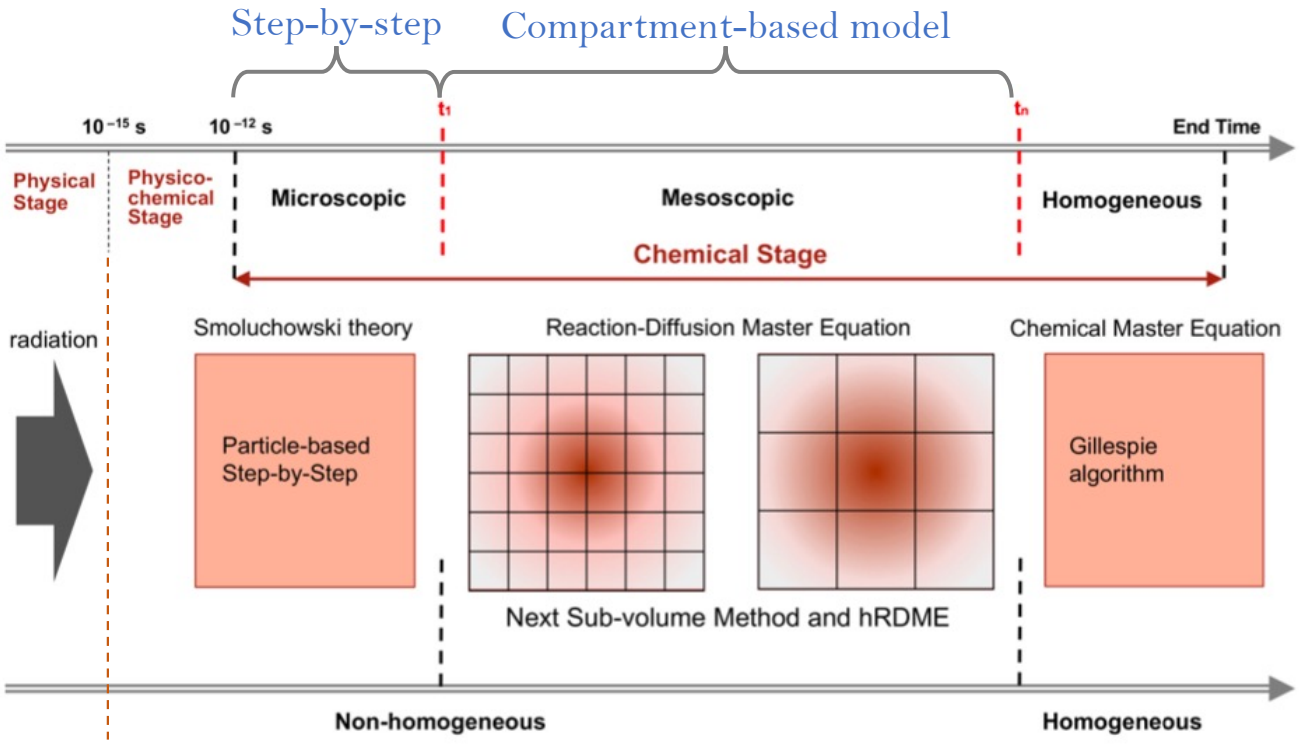
5 µm^3 water cube
Conventional dose rate
PhaseSpace around the cube.
PhaseSpace source in HDF5 format.



H_2O_2 G values along time, using 3 physics lists



Water radiolysis beyond the microsecond for UHDR protons



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?

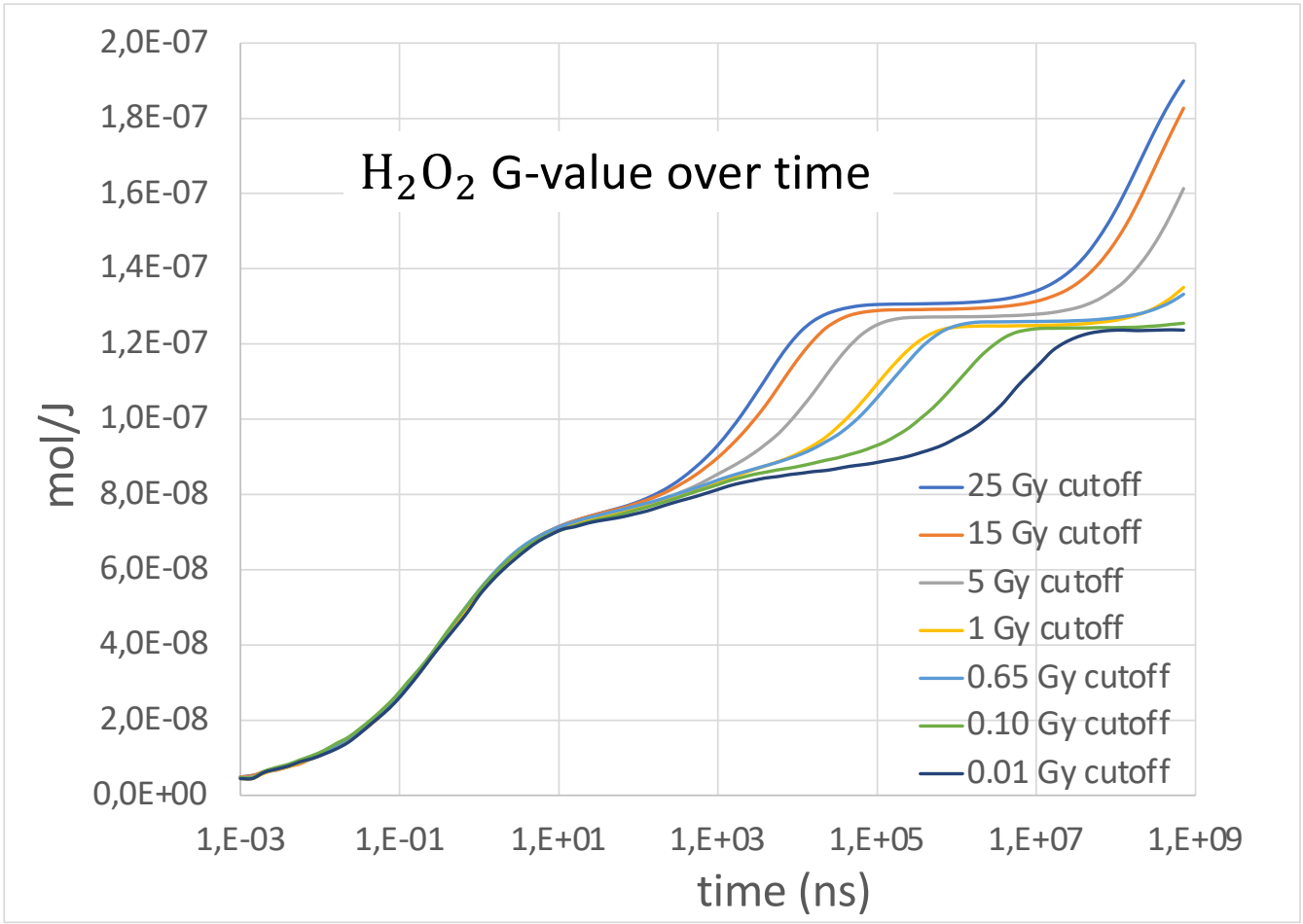
Protons are generated till a cutoff dose is reached

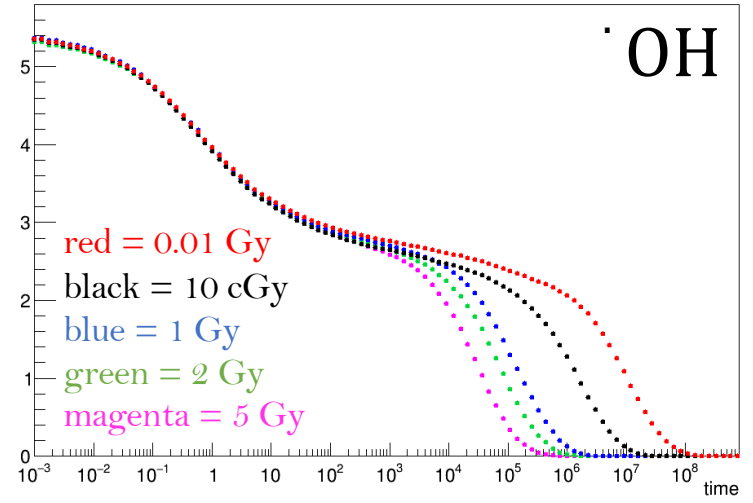
Tran,H.N.;Chappuis,F.; Incerti, S.; Bochud, F.; Desorgher, L.
Geant4-DNA Modeling of Water Radiolysis beyond the Microsecond: An On-Lattice Stochastic Approach.
Int. J. Mol. Sci. **2021**, *22*, 6023. https://doi.org/10.3390/ ijms22116023

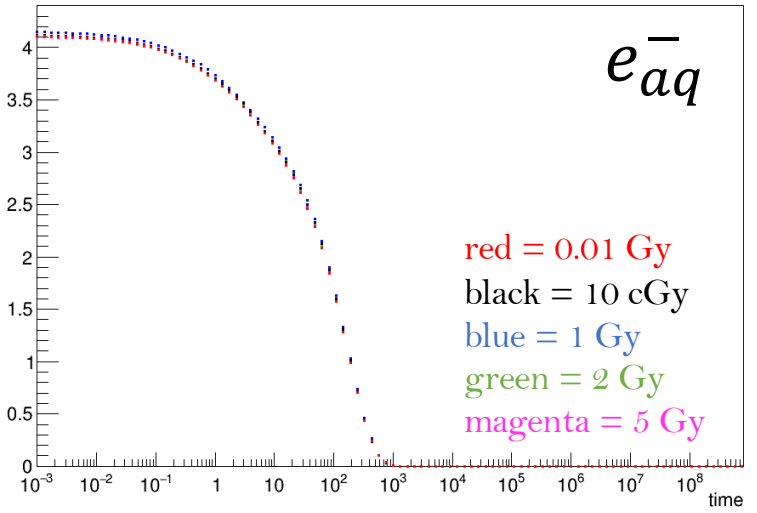
Results – Aerated water

57 MeV protons

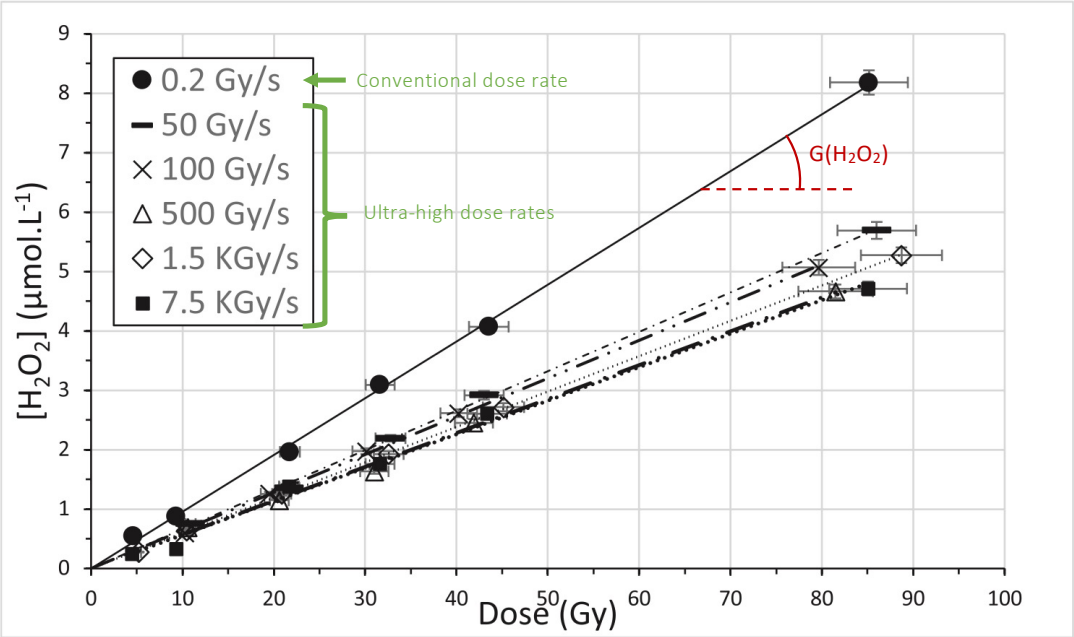
➢ In **aerated environment** H_2O_2 production depends on the dose per pulse







Experimental measurements



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

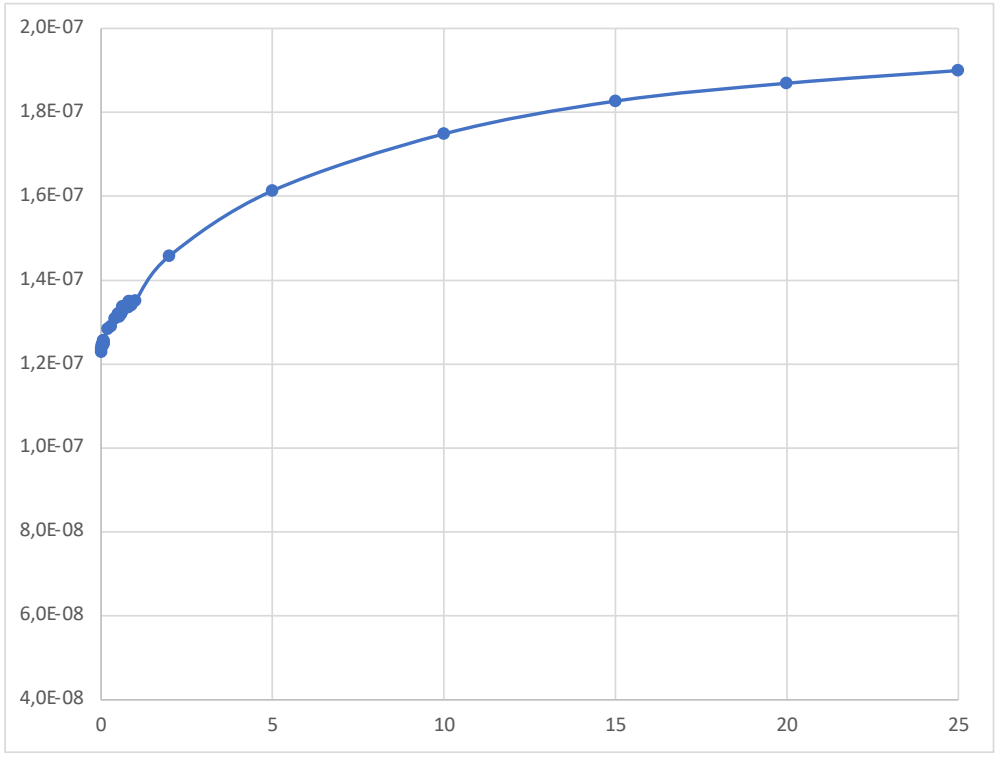
The concentration of H_2O_2 was obtained indirectly by measurement of I_3^- absorbance using a spectrophotometer.

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

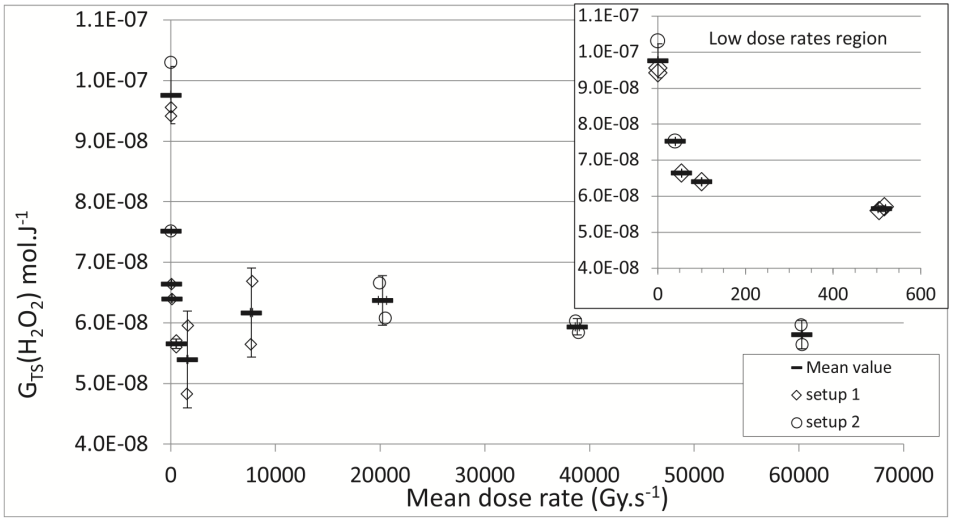
Blain,G. et al.
Proton Irradiation at Ultra-High Dose Rate vs. Conventional Dose Rate: Strong Impact on Hydrogen Peroxide Yield.
Radiation Research, **2022**, *198*, 318-324.

Simulations vs experimental measurements

G4-DNA simulations



Experience

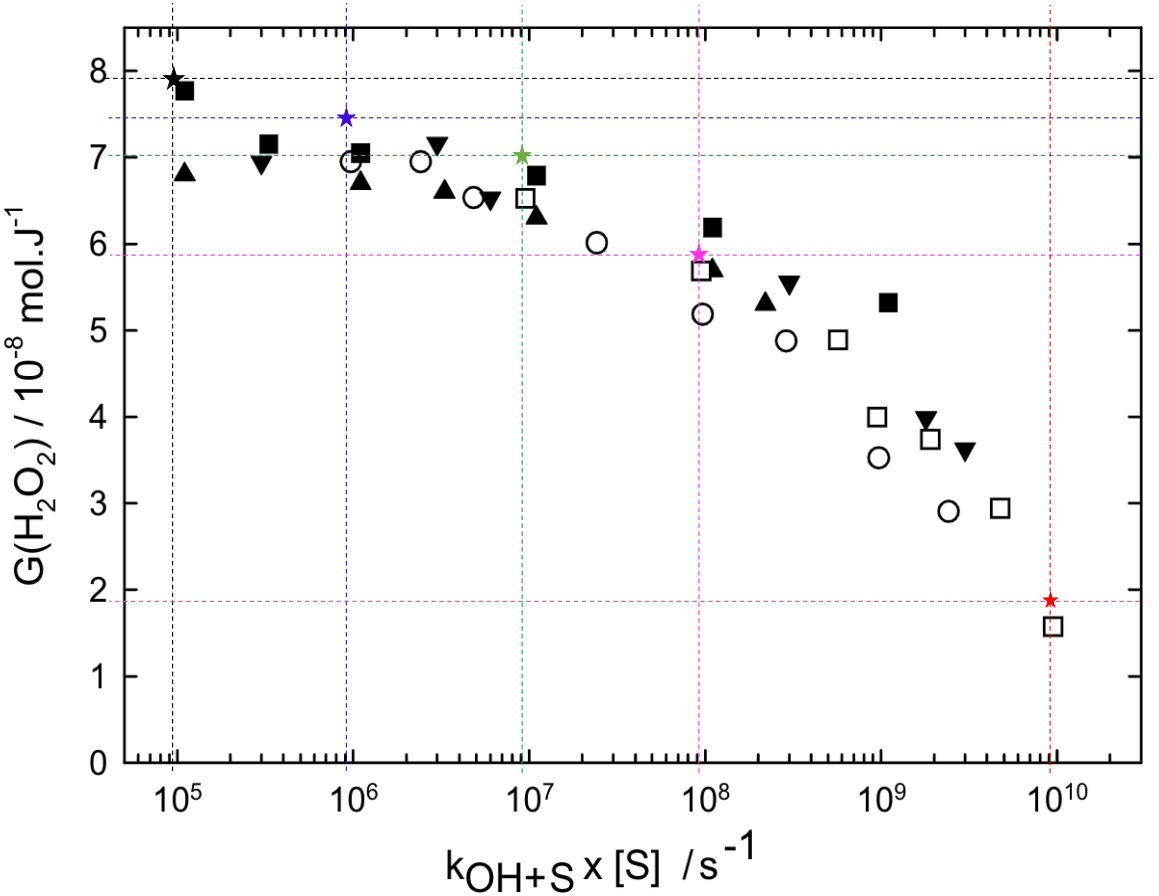


Blain,G. et al.
Proton Irradiation at Ultra-High Dose Rate vs. Conventional Dose Rate: Strong Impact on Hydrogen Peroxide Yield.
Radiation Research, **2022**, *198*, 318-324.

Hypothesis:
- **pH variation**
- **Longer time**

NO2 scavenger validation

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



$$OH + NO_2^- \rightarrow NO_2 + OH^-$$

k=8e9 $M^{-1}s^{-1}$

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

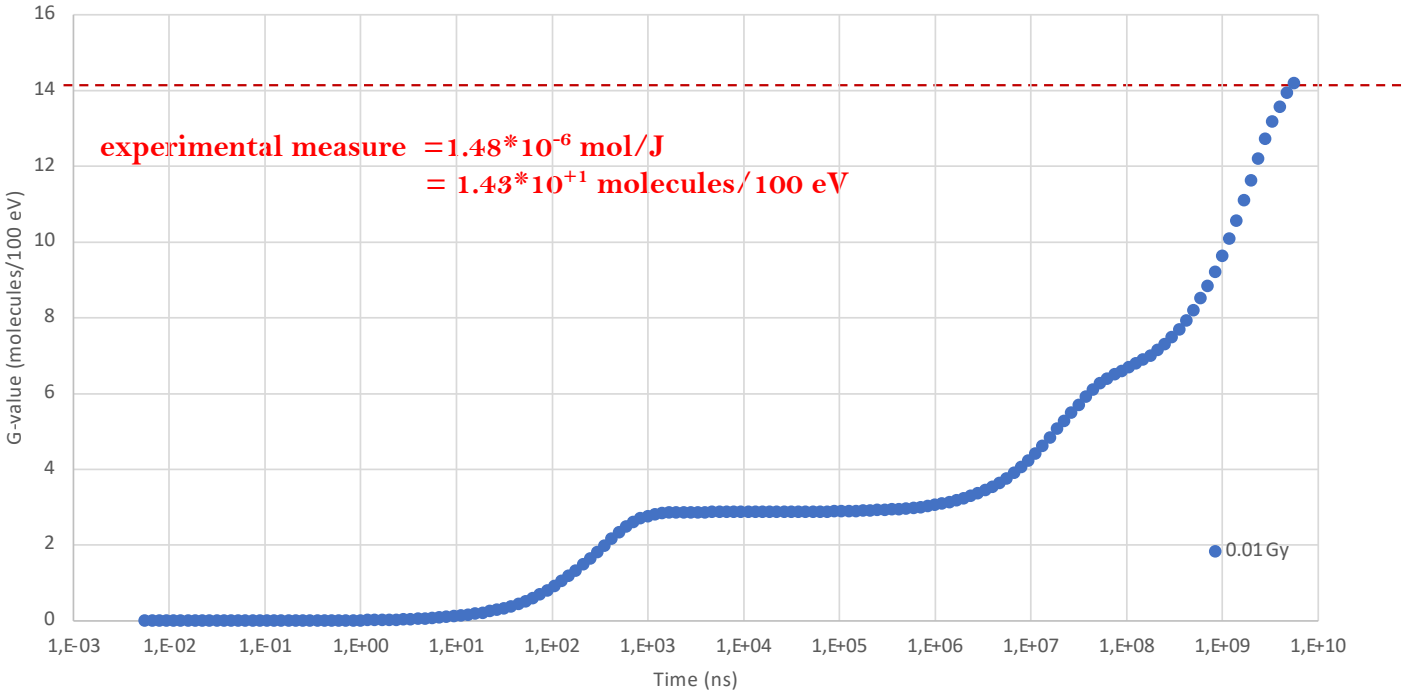
Wasselin-Trupin· Baldacchino. Bouffard. Hickel

Radiation Physics and Chemistry

Volume 65, Issue 1, August 2002, Pages 53-61

Fricke dosimeter

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

$$Fe^{2+} + {}^{\cdot}OH \rightarrow Fe^{3+} + {}^{\cdot}OH^{-}$$

$$Fe^{2+} + HO_2 \rightarrow Fe^{3+} + HO_2^{-}$$

$$Fe^{2+} + H_2O_2 \rightarrow Fe^{3+} + {}^{\cdot}OH + OH^{-}$$

Added scavengers:

```
/chem/env/Scavenger O2 19 %
/chem/env/Scavenger Fepp 10 mM
```

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 ≠ 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