Unlocking radiolysis: gMicroMC's leap from micro to macro simulations and the B-yield's key role in CONV vs. FLASH

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M. Molina-Hernandez[1,2,3], Y. Chi[4], P. Gonçalves[2,3], J. Seco[1,5]

[1]German Cancer Research Center, Biomedical Physics in Radiation Oncology (E041), Heidelberg, Germany, [2]Laboratory of Instrumentation and Experimental Particles Physics, LIP, Lisboa, Portugal, [3]University Técnico Lisboa, Physical Engineering, Lisboa, Portugal, [4]University of Texas at Arlington, Physics Research & Techniques in Radiation Medicine, Arlington, United States of America, [5]University of Heidelberg, Physics and Astronomy, Heidelberg, Germany

Introduction

Extensive studies on the macroscopic G-yield indicate dose rate dependencies: during FLASH, the O_2 depletion rate decreases, while the H_2O_2 concentration is reduced. The goal of this research is to broaden the scope of gMicroMC beyond the traditional microscopic analysis of individual radiation tracks to include the simulation of pulsed beams. The advancement involves shifting towards simulating a macroscopic phenomenon as a pulsed irradiation is, encompassing macroscopic inputs such as dose, dose rate and beam structure. Ultimately, we aim at grasping the radiochemical distinctions between CONV vs. FLASH.

Methods

We developed a pulse irradiation model (PIM), which stands on three pillars. Firstly, gMicroMC's step-by-step (SBS) algorithm, which dissociation schemes, branching ratios and chemistry lists were updated. The Periodic Boundary Condition (PBC), which ensures that that microscopic simulated system reflects the larger, macroscopic, bulk properties. To efficiently track the chemicals over extended periods, we included Numerical Ordinary Differential Equations (NumODEs), which were validated against Kinetiscope. We define a $\dot{D}_{av}$ threshold for every $\dot{D}_p$. Below the threshold (CONV), the G-yield is constant; above it (FLASH), the G-yield depends on the $\dot{D}_{av}$.

Results

We reproduced a pulse radiolysis experiment characterized by a pulse with FWHM = 1 µs delivering 1 Gy. Figure 1 shows the primary G-yield as an LET function and experimental measurements. Additionally, we irradiated pure water to a total dose of 20 Gy using a 70 MeV proton beam characterized by pulses with a duration of 1 µs. Figure 2 shows the G-yield of H_2O_2 as a $\dot{D}_{av}$ function. For $\dot{D}_p$ of $1.8\cdot10^5$ and 10^6 Gy/s, the $\dot{D}_{av}$ thresholds were observed at ~10 Gy/s and ~100 Gy/s, respectively. In Figure 3, at the inception of every pulse, it can be observed a background yield (B-yield) of chemicals. For CONV, the B-yield is constituted by H_2 and H_2O_2, whereas for FLASH, it is a mixture of all the species.

Conclusions

Our PIM is the first model to bridge the gap between the microscopic and macroscopic realms. The B-yield determines the $\dot{D}_{av}$ threshold and, consequently the dependence of the G-yield with $\dot{D}_p$ and $\dot{D}_{av}$. Furthermore, the B-yield theory provides a better understanding of the dose rate dependencies over the inter-tracking theory. The FLASH effect has been demonstrated with comparable $\dot{D}_{av}$ thresholds for identical $\dot{D}_p$. Our findings suggest a potential correlation between the FLASH effect and radiochemistry.

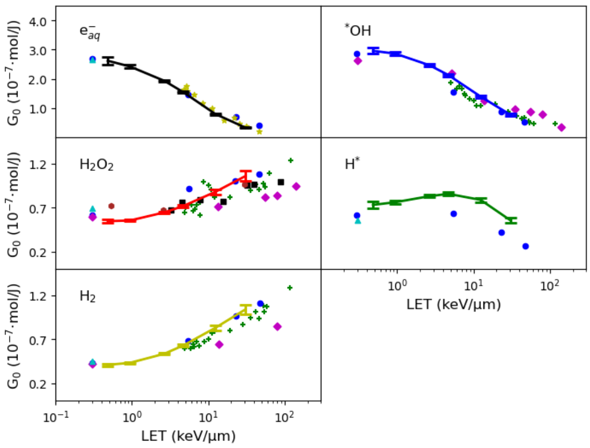

Figure 1: Primary G-yield (G_0) as an LET function for a pulse with FWHM = 1 μs and delivering 1 Gy and experimental measurements.

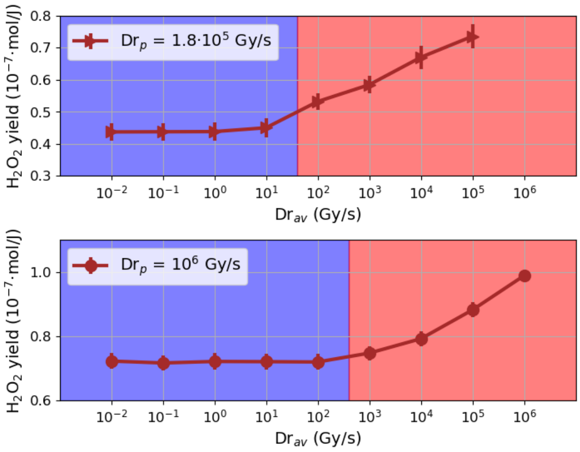

Figure 2: H_2O_2 yield for $\dot{D}_p$ of $1.8 \cdot 10^5$ Gy/s and 10^6 Gy/s as a $\dot{D}_p$ function. CONV in blue and FLASH in red.

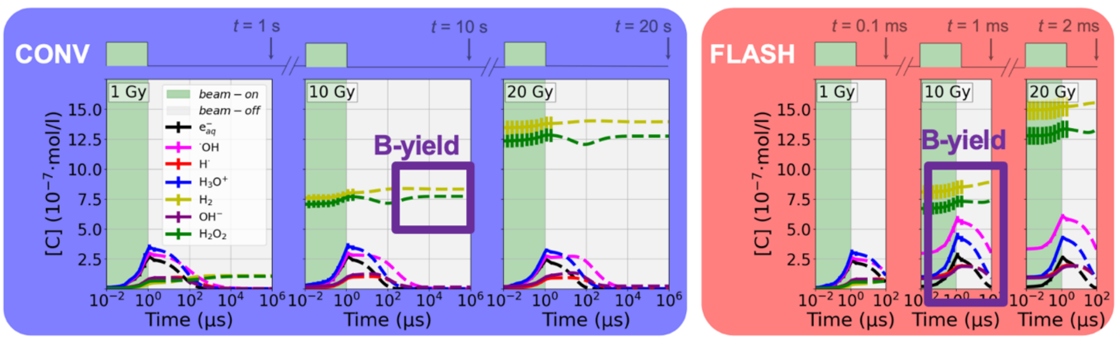

Figure 3: Species concentration time evolution during pulses for CONV ($\dot{D}_p = 10^6$ Gy/s and $\dot{D}_{av} = 10$ Gy/s) and FLASH ($\dot{D}_p = 10^6$ Gy/s and $\dot{D}_{av} = 10000$ Gy/s). The SBS figures as error bars and the NumODEs as dashed lines.