Effects of the Oxygen depletion in extremely high dose rate proton irradiation investigated through Scavenger example

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Outlook:

- High dose rate irradiation & Oxygen Effects
- High dose rate irradiation & Scavenger Example

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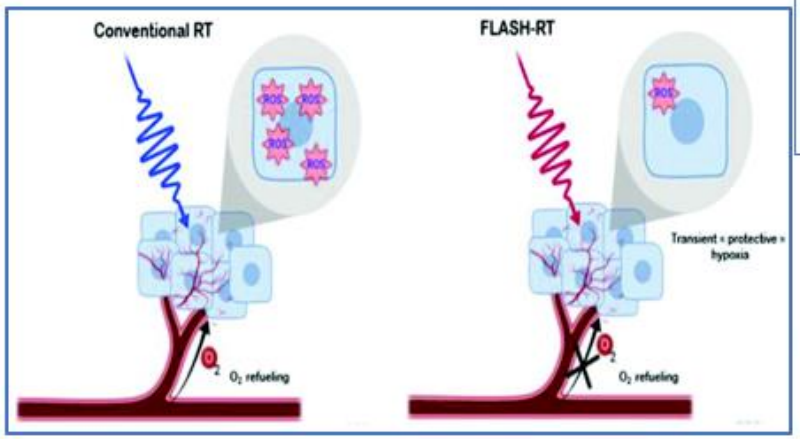
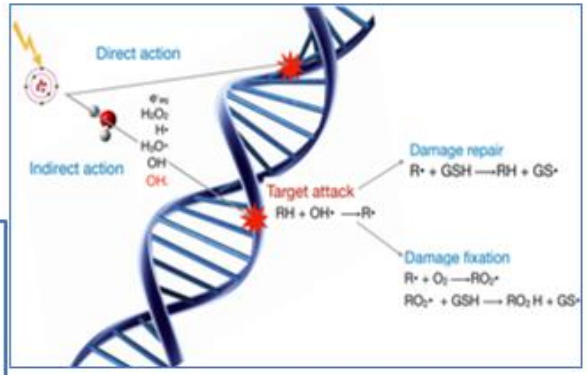
High dose rate irradiation & Oxygen Effects

General Idea

Cells are much more sensitive to irradiation in the presence of molecular oxygen.

$$e^-_{aq} + O_2 \longrightarrow O_2^{\bullet -}$$
$$H^{\bullet} + O_2 \longrightarrow HO_2^{\bullet}.$$





the oxygen fixation hypothesis

$$OER(pO_2) = \frac{D_{pO_2}}{D_{\text{normoxic}}}\Big|_{\text{same effect}}$$

- **OER factor** indicates the **level of radio sensitivity** due to **the presence of oxygen.**

High dose rate irradiation & Scavenger Example

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Limitations

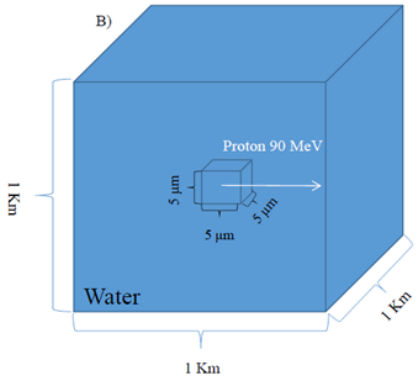
Geant4-DNA is a set of libraries to simulate the transport and the energy depositions of ionizing radiation in **biological materials such as water and DNA.**

Simulation of **the oxygen diffusion from air to water target** (in order to calculate of oxygen concentration).

Solutions

In the physical stage, the box material is water, while **for the chemical one, it is: water + a specific oxygen concentration** through an **external file** defining the possible chemical reactions and the oxygen concentration.

We assumed dissolved oxygen molecules as a **continuum backdrop**, with a constant **diffusion rate of zero** by considering **reactions type VI**.



condition:

The irradiated water box is **sealed** (**isolated from oxygen**)

It is NOT possible to **reoxygenate** from outside the target during the short radiation pulse (µs).

```
scavenger: O2     27e-05  # 21% in partial pressure


# Reactions between radio-induced species --------------------
# REACTANTS -> PRODUCTS , RATE [1/s/(mole/l)] or [1/s]   TYPE
#-------------------------------------------------------------
e_aq + e_aq + [H2O] + [H2O] -> H2 + OH- + OH- , 6.36e9      type_3
e_aq + OH -> OH- ,                              2.95e10     type_2
e_aq + H + [H2O] -> H2 + OH- ,                  2.50e10     type_1
e_aq + H3O+ -> H + [H2O] ,                      2.11e10     type_4
e_aq + H2O2 -> OH- + OH ,                       1.10e10     type_2
OH + OH -> H2O2 ,                               5.50e9      type_2
OH + H -> [H2O] ,                               1.55e10     type_2
H + H -> H2 ,                                   5.03e9      type_1
H3O+ + OH- -> [H2O] + [H2O] ,                   1.13e11     type_3
H + HO2 -> H2O2 ,                               1.00e10     type_2
H + O2- -> HO2- ,                               1.00e10     type_2
OH + HO2 -> O2 ,                                7.90e9      type_2
OH + O2- -> O2 + OH- ,                          1.07e10     type_2
OH + HO2- -> HO2 + OH- ,                        8.32e9      type_2
e_aq + HO2 -> HO2- ,                            1.29e10     type_2
HO2 + HO2 -> H2O2 + O2 ,                        9.80e5      type_2
HO2 + O2- -> HO2- + O2 ,                        9.70e7      type_2
e_aq + O2- -> H2O2 + OH- + OH- ,                1.29e10     type_4
H3O+ + O2- -> HO2 ,                             4.78e10     type_4
H3O+ + HO2- -> H2O2 ,                           5.00e10     type_4


# Reactions with the scavengers
# Specify the scavenger with []
#------------------------------
e_aq + [O2] -> O2- , 1.74e10    type_6
H + [O2] -> HO2 ,    2.10e10    type_6
O- + [O2] -> O3- ,   3.70e9     type_6
```

External file

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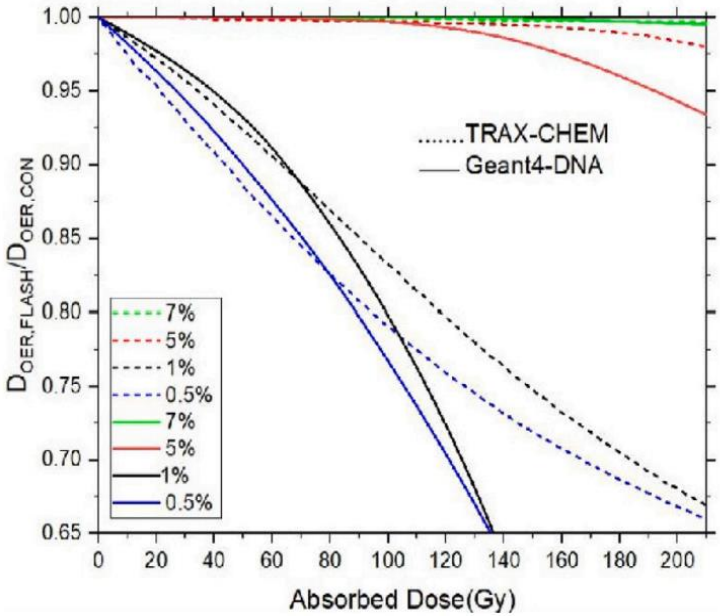
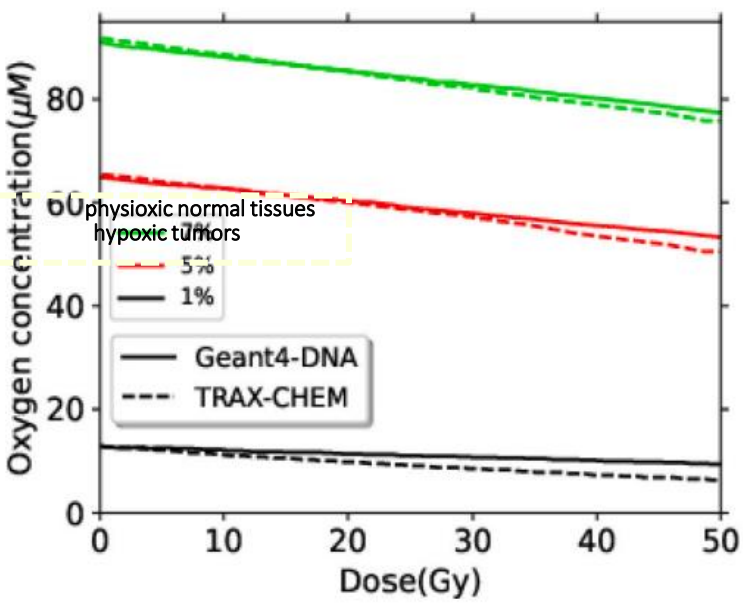
Oxygen concentration vs. Dose

Oxygen concentration as a **function of dose** under extremely high dose rate irradiation with $\mathbf{1}\boldsymbol{MeV}$ electrons at various initial oxygenations, in comparison with the TRAX-CHEM code results.





1) Oxygen reduction is not observed in the range of clinical doses.

2) Complete depletion is not observed for any initial oxygen concentration.

FINDINGS

F Farokhi et al., Radiation Physics and Chemistry 212 (2023) 111184

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Concolusions:

1. Using **Geant4-DNA** and **OER index**, specifically for low LET radiation, we have shown that **oxygen depletion is not observed in the range of clinical doses**.

2. Although Geant4-DNA toolkit, as one of the Monte Carlo track structure codes, is suited for this class of simulation, further improvements are needed in the chemical stage and specific chemical interactions that should be considered.

Future development

Limitation of Scavenger → what we want to improve:

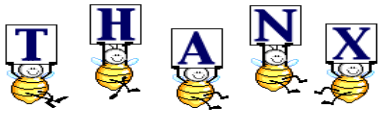
1- Modeling of Water Radiolysis beyond the Microsecond to minutes.

2- Including the fact of pH in presence of different oxygen concentrations.

3- Considering the pulse time structure.

See presentation → " UHDR example: overview, updates & perspectives",
Serena Fattori on behalf of the Geant4-DNA Collaboration.

Thank you for your attention



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