Overview of pre-chemical aspects of Geant4-DNA and initial radiological yields

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Representing the efforts of the Geant4-DNA Collaboration

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Monte Carlo track structure (MCTS) codes typically approximate biological medium as liquid water, which composes more than 60% of human body.

In addition, the number of indirect strand breaks is dominant particularly at low linear energy transfer (LET).

Thus, a careful study of radiochemical yield simulation in liquid water under MeV electron irradiation is of strong interest.
This stage determines the number (and distribution) of chemical species induced by physical interactions at early time (1 ps).

However, it is still impossible to understand mechanistically femtosecond-scale aspects of pre-chemical stage.

Thus, the pre-chemical parameters are adjusted for calculating G-values to match experimental data in this study.
1) Thermalization of electrons (primaries and secondaries)
   - $e^{-} (< 10 \text{ eV}) \rightarrow e^{-} (0.025 \text{ eV}) \rightarrow e_{aq}^{-}$

2) Physico-chemical interactions
   - Auger effect
     - $H_2O + e^{-} \rightarrow H_2O^{2+} + 3e^{-}$
   - Electron dissociative attachment
     - $H_2O + e^{-} \rightarrow H_2O^{-}$
   - Electron-hole recombination
     - $H_2O^{+} + e_{aq}^{-} \rightarrow H_2O^{*}$

3) Dissociation of ionized and excited water molecules
   - e.g.) $H_2O^{+} \rightarrow H^{+} + OH$
To find out the optimal pre-chemical model for water radiolysis

The models used in Geant4-DNA are corrected in order to be consistent with original papers

1) Electron thermalization model
2) Physico-chemical interactions
3) Dissociation channels
1) Electron thermalization model

- Tracking very low energy electrons (<10 eV, “sub-excitation electrons”) is a huge burden.
- MCTS codes usually simulate in one step the distance travelled by electrons until thermalization.

2) Physico-chemical interactions

- Auger effect
  - Generates two electrons and one $\text{H}_2\text{O}^{2+}$ instead of $\text{H}_2\text{O}^+$
  - The dissociation channel of $\text{H}_2\text{O}^{2+}$ is taken into account.

- Electron dissociative attachment
  - Bug fix on cut-off dependency

- Electron-hole recombination
  - Modify the dissociation channel
3) History of dissociation model

- Cobut et al. (1998), TRACELE and TRACPRO
  - Adjust B\(^1\)A\(_1\) excitation
  - Add Rydberg excitation
  - Except attachment and recombination
  - Adjustable

- Kreipl et al. (2009), PARTRAC
  - Copy the values
  - Add attachment and recombination

- Karamitros et al. (2011), Geant4-DNA

- Plante (2011), RITRACKS
### Dissociation channel

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- Physical interactions

- The observed discontinuities up to 30% between electron-proton-alpha cases are due to the different physics models.

- The contribution of Auger effect is indeed much smaller.
The G-values of *OH radicals calculated in this study are closer to recent experimental data such as the ones of Wang et al (2018).
The main improvement here is that the G-values of $\text{H}_2\text{O}_2$, which previously showed higher values than the literature data using the public version of Geant4-DNA.
Conclusions

- In this study, we find out the optimal electron thermalization, electron attachment, and electron-hole recombination models. In addition, the dissociation model is modified based on the original works of the model.

- The influence of those corrections is about 4% on •OH radical at 1 ps, and the calculated G-values are within the experimental errors of the most recent data.

- Especially, the number of H$_2$O$_2$ generated by •OH+ •OH reactions become closer to the experimental data on G versus LET results.

- These improvements will soon be supplemented as G4EmDNAChemistry_option3 constructor in Geant4.

Thank you very much for your attention!