Introduction

The irradiation of biological systems leads to the formation of radiolytic species such as H\textsubscript{2}, OH, H\textsubscript{2}O\textsubscript{2}, e\textsubscript{aq} etc. [1]. These species react with neighboring molecules, which result in damage in biological molecules such as DNA.

Radiation chemistry is therefore very important to understand the radiobiological consequences of radiation [2]. In this work, we discuss an approach based on the exact Green Functions for diffusion-influenced reactions which may be used to simulate radiation chemistry and eventually extended to study more complex systems, including DNA.

Green functions

The exact Green functions for an isolated pair are known analytically [3-4]:

\begin{align*}
\psi(r,t|\tau_0) &= \frac{1}{\sqrt{4\pi \tau_0}} \exp\left(-\frac{r^2}{4\tau_0}\right) \\
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\end{align*}

The coefficients \(\alpha, \beta\) and \(\gamma\) are related to the reaction rate constants \(k_0=4\pi RD\): \(\alpha + \beta + \gamma = 1 + k_1/k_2, D\)

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Chemical reactions and radiolytic yields

The chemical reactions between radiolytic species with no electrostatic interaction (i.e. their charge product is 0) can be simulated by using the Green Functions described above.

The radiation chemistry code can be used to simulate the time evolution of the radiolytic species (radiation chemistry) and radiochemical yields [5,6].

Assumptions of the model

- The pair of particle may react as follow [3]:

\[
A + B \rightarrow (AB) \rightarrow AB
\]

\[
k_+ \text{ association rate constant} \\
k_- \text{ dissociation rate constant} \\
k_\text{p} \text{ product formation rate constant}
\]

- Transitions from a state to another are defined:

<table>
<thead>
<tr>
<th>Initial state</th>
<th>Free ((k_0))</th>
<th>Rev bound ((k_1))</th>
<th>Products ((k_2))</th>
</tr>
</thead>
<tbody>
<tr>
<td>(k_0)</td>
<td>(k_0(1-k))</td>
<td>(k_0(1-k))</td>
<td>(k_0(1-k))</td>
</tr>
<tr>
<td>Rev bound</td>
<td>(k_1(1-k))</td>
<td>(k_1(1-k))</td>
<td>(k_1(1-k))</td>
</tr>
<tr>
<td>Products</td>
<td>0</td>
<td>0</td>
<td>1</td>
</tr>
</tbody>
</table>

Sampling of the Green functions

- We have developed exact algorithms to sample the random variables \(r\) for \(p(r,|t_0)\) and \(p(t,|t_0)\) [4].

- The algorithm allow the simulation to be done in several timesteps (time discretization)

\[
\begin{align*}
\text{Left: Green function } &4\pi(\psi(r,t|\tau_0)) \text{ for } R=1, \tau_0=1.5, \text{ for } k_0=4.0R, k_1=1.0, \text{ and } k_2=1.0 \text{ at } t=1, 2, 4, 8, 16, \text{ and } 32. \\
\text{Analytical functions: } &\text{(--) Result of sampling; (w) Right Survival probability } Q(t,\tau_0) \text{, binding probability } p^t(\tau_0) \text{ and reaction probability } p^r(\tau_0) \text{ as function of time for } R=1, \tau_0=1.5, k_0=4.0R, k_1=1.0, \text{ and } k_2=1.0. \\
\text{Right: Survival probability: } &Q(t,\tau_0) = 4\pi \tau_0 p(t,|\tau_0)
\end{align*}
\]

Radiation track structure and evolution in time

- This approach has been used successfully to simulate the time evolution of radiolytic species and to calculate radiochemical yields.

- The radiation track structure code RITRACKS [7] and the chemistry code will be of crucial importance in future models of DNA damage.

References