A radiation chemistry code based on the Green’s functions of the Diffusion Equation

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The space radiation problem

- Space radiation is comprised of high-energy protons and heavy ions (HZE’s) and secondary protons, neutrons, and heavy ions produced in shielding.

- Unique damage to biomolecules, cells, and tissues occurs from HZE ions that is qualitatively distinct from X-rays and gamma-rays on Earth.

- No human data to estimate risk from heavy ions, thus requiring use of biological models and theoretical understanding to assess and mitigate risks.

- Shielding has excessive costs and will not eliminate galactic cosmic rays (GCR).

Radiation tracks and energy deposition

- The energy deposition by heavy ions is highly heterogeneous and dependent on the type and energy of the ion.
- The interactions of radiation with matter are stochastic in nature and therefore often studied by Monte-Carlo simulations.

Primary energy loss events in low-LET tracks

Primary energy loss events in high-LET tracks

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## Radiation effects: time sequence of events

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<th>Modeling</th>
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</table>
Radiation effects: time sequence of events

$\text{H}_2\text{O}$

Physical stage (<$10^{-15}$ s)

Physico-Chemical stage ($\sim 10^{-15} - 10^{-12}$ s)

$\text{H}_2\text{O} + \text{H}_2\text{O}^* + e^- \rightarrow \text{H}_2\text{O}^* + \text{H}_2\text{O}$

$\text{H}_2\text{O}^* \rightarrow \text{H}_2 + \text{O}^{{1D}}$

$2 \text{H}^* + \text{O}^{{3P}}$

$\text{e}^-_{\text{aq}} \rightarrow \text{H}_2 + \text{OH}^-$

$\sim 240-600$ fs
Particle transport basics

- The trajectory of a particle and all its interactions is followed in the medium.

- Many other particles are generated by the interactions of the “primary” particle. The trajectories of these secondary particles should also be followed.

- A particle is followed until:
  - Its energy decrease below a threshold
  - It disappears by a physical process (e.g. absorption of a photon during a photo-electric effect)
  - It leaves the volume of interest

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Particle transport basics

- **Particles**
  - Position (x,y,z)
  - Energy (E)
  - Direction (θ,φ)

- **Cross sections**
  - Probability of interaction between radiation and matter

\[
\frac{dI}{dx} = -I n \sigma dx
\]

- **Cross sections** (units: \(\text{cm}^2\))
- **Mean free path** \(\lambda\) (units: cm)

\[
\lambda(E) = \frac{1}{N\sigma(E)}
\]

\[
I(x) = I(0) \exp(-x / \lambda(E))
\]
Cross sections

- Cross sections (total and differential in energy, angle, … i.e. d\(\sigma/dW\), d\(\sigma/d\theta\), d\(^{2}\sigma/dWd\sigma\), …) are needed for particle transport.

- RITRACKS includes accurate cross section models for all ions and secondary electrons or photons.

- For electrons:
  - Ionization
  - Excitation
  - Elastic collisions
  - Dissociative electron attachment
  - Bremsstrahlung

- For ions:
  - Ionization
  - Excitation

- For photons:
  - Compton effect
  - Coherent diffusion
  - Photoelectric effect
  - Pair production

Cross sections used in RITRACKS

The cross sections for ions are scaled with $Z_{\text{eff}}$:

$$\frac{d\sigma_{\text{ion}}(v)}{dW} = Z_{\text{eff}}^2 \frac{d\sigma_{\text{proton}}(v)}{dW}$$

$$Z_{\text{eff}} / Z = 1 - \exp(-125\beta^2 / Z^{2/3})$$

$v$: velocity of the ion

$\beta$: relativistic $v/c$
Heavy ion track structure simulation

Simulation for $^1\text{H}^+$, $^{12}\text{C}^{6+}$, $^{28}\text{Si}^{14+}$ and $^{56}\text{Fe}^{26+}$ tracks, 100 MeV/amu
Radial dosimetry

(a) $^1$H$^+$ 1 MeV/amu, LET~33 keV/μm
(b) $^{20}$Ne$^{10+}$ 377 MeV/amu, LET~31 keV/μm
(c) $^4$He$^{2+}$ 1 MeV/amu, $^{56}$Fe$^{26+}$ 1 GeV/amu, LET~150 keV/μm

Voxel dosimetry

1 GeV/amu $^{56}$Fe$^{26+}$ ion
LET $\sim$ 150 keV/$\mu$m
Voxels: 40 nm x 40 nm x 40 nm

DNA damage / $\gamma$H2AX foci studies

- Irradiation by 1 GeV/amu Fe ions
- 100 cGy
- LET $\sim$ 149 keV/$\mu$m

Experiments performed at the NASA Space Radiation Laboratory (2007)
DNA damage

2700 x $^1\text{H}^+$, 300 MeV (1 Gy)
Dose in voxels (20 nm)
Chromosomes (RW model)
Intersection voxels
H2AX foci experiments
Application of DSB probability

$$\psi = 1 - e^{-QD(t)}$$
DNA damage

6 x $^{56}\text{Fe}^{26+}$, 1 GeV/u (1 Gy)
Dose in voxels (20 nm)
Chromosomes (RW model)
Intersection voxels
H2AX foci experiments
Application of DSB probability

$$\psi = 1 - e^{-QD(t)}$$

DNA damage / $\gamma$H2AX foci studies

- Calculation of DSBs by low- and high-LET radiation

DNA damage / $\gamma$H2AX foci studies

- Calculation of DSBs by $^1$H$^+$, $^{12}$C$^{6+}$ and $^{56}$Fe$^{26+}$ ions

DNA damage / γH2AX foci studies

• Calculation of DSBs vs LET by $^1\text{H}^+$, $^{12}\text{C}^{6+}$ and $^{56}\text{Fe}^{26+}$ ions

To better understand the formation of DSBs, a chromatin fiber is build from nucleosome units and linker DNA.
The Binary-Encounter-Bethe (BEB) model of ionization cross section

\[
\frac{d\sigma}{dw} = \frac{s}{t+u+1} \left\{ \frac{1}{(t-w)^2} + \frac{1}{(1+w)^2} - \frac{1}{1+t} \left[ \frac{1}{t-w} + \frac{1}{1+w} \right] + \frac{1}{(t-w)^3} + \frac{1}{(1+w)^3} \right\} \log(t) \right\}
\]

The energies are expressed in units of ionization potential of the orbital (B):

- t=T/B is the kinetic energy of the incident electron
- w=W/B is the kinetic energy of the ejected electron
- u=U/B is the kinetic energy of the electron in the orbital

The total cross section is obtained by integration

\[
\sigma = \left( \frac{t-1}{2} \right)^2 \int_0^\infty \frac{d\sigma}{dw} dw = \frac{s}{t+u+1} \left\{ 1 - \frac{1}{t} + \frac{1}{2} \left[ 1 - \frac{1}{t^2} \right] \log(t) - \frac{\log(t)}{t+1} \right\}
\]

In the DNA bases, there are many internal and valence electrons. The BEB model allows to model the ionization for each electron of the molecule.

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Thymine calculations from the site www.chemeddl.org

DNA damage simulations

Calculations of MO from the site www.chemeddl.org
DNA damage studies

- Cross sections can be calculated for the bases, sugars and phosphates.
- In this case, the medium is considered a succession of homogeneous media.

\[ dI = -\ln N \sigma dx \]

\[ \ln \left( \frac{I}{I_0} \right) = -\int_0^x \sigma(u) N du \]

\[ I = I_0 \exp \left\{ -N \left[ \sum_{j=1}^{i-1} (\sigma_j - \sigma_i) W_j + \sigma_i x \right] \right\} \]

Relative weight

\[ p_i = I_0 \frac{\exp(-N \sum_{j=1}^{i-1} W_j \sigma_j)(1 - \exp(-NW_i \sigma_i))}{N \sigma_i} \]

Sampling of \( W_s \)

\[ W_s = \sum_{j=1}^{i-1} W_j - \frac{1}{N \sigma_i} \log \left[ 1 - V(1 - e^{-\sigma_i NW_j}) \right] \]

Radiation chemistry

- $\sim 10^{-12} - 10^{-6}$ s
  - Particles diffusion
  - Chemical reactions

- The radiolytic species are not uniformly distributed. Therefore, an approach based on Green’s functions of the diffusion equation (DE) is used.

Examples of chemical reactions:

\[ \text{e}^{-}_{\text{aq}} + \text{e}^{-}_{\text{aq}} \xrightarrow{2\text{H}_2\text{O}} \text{H}_2 + 2 \text{OH}^- \]

\[ \cdot\text{OH} + \text{e}^{-}_{\text{aq}} \rightarrow \text{OH}^- \]

\[ \cdot\text{OH} + \cdot\text{OH} \rightarrow \text{H}_2\text{O}_2 \]

\[ \cdot\text{OH} + \text{H}_2\text{O}_2 \rightarrow \text{HO}_2^\cdot + \text{H}_2\text{O} \]

\[ \text{H}^+ + \text{O}_2^- \leftrightarrow \text{HO}_2^\cdot \]

\[ \text{H}^\cdot + \text{H}_2\text{O}_2 \rightarrow \cdot\text{OH} + \text{H}_2\text{O} \]

(Number of chemical species created)

\[ G(X) = \frac{100 \text{ eV deposited energy}}{} \]
Bimolecular reactions

- DE for the propagation of particles A and B

\[
\frac{\partial p(r_A, r_B, t | r_{A0}, r_{B0}, t_0)}{\partial t} = \left[ D_A \nabla_A^2 + D_B \nabla_B^2 \right] p(r_A, r_B, t | r_{A0}, r_{B0}, t_0)
\]

- Transformation

\[
R = \sqrt{\frac{D_B}{D_A}} r_A + \sqrt{\frac{D_A}{D_B}} r_B \quad \nabla_R = \frac{\partial}{\partial R} \\
r = r_B - r_A \quad \nabla_r = \frac{\partial}{\partial r}
\]

\[
\frac{\partial p(R, r, t | R_0, r_0, t_0)}{\partial t} = \left( D_A + D_B \right) \left[ \nabla_R^2 + \nabla_r^2 \right] p(R, r, t | R_0, r_0, t_0)
\]

\[p(R, r, t | R_0, r_0, t_0) = p^R(R, t | R_0, t_0)p^r(r, t | r_0, t_0)
\]

\[
\frac{\partial p^R(R, t | R_0, t_0)}{\partial t} = \left( D_A + D_B \right) \nabla_R^2 p^R(R, t | R_0, t_0)
\]

\[
\frac{\partial p^r(r, t | r_0, t_0)}{\partial t} = \left( D_A + D_B \right) \nabla_r^2 p^r(r, t | r_0, t_0)
\]

p(R, r, t | r_{A0}, r_{B0}, t_0): probability of particles A and B to be at positions r_A and r_B at time t, given that they were at r_{A0} and r_{B0} at t_0

D_A, D_B: Diffusion coefficients

Uncoupled equations

in \( r \) and \( R \)

Free diffusive motion of the coordinate $\mathbf{R}$

$$\frac{\partial p^R (\mathbf{R}, t \mid \mathbf{R}_0, t_0)}{\partial t} = D \nabla_R^2 p^R (\mathbf{R}, t \mid \mathbf{R}_0, t_0)$$  \hspace{1cm} \text{(DE)}$$

$$p^R (\mathbf{R}, t \mid \mathbf{R}_0, t_0) = \delta (\mathbf{R} - \mathbf{R}_0)$$  \hspace{1cm} \text{(Initial condition)}$$

$$p^R (|\mathbf{R}| \to \infty, t \mid \mathbf{R}_0, t_0) = 0$$  \hspace{1cm} \text{(Boundary condition)}$$

$$p^R (\mathbf{R}, t \mid \mathbf{R}_0, t_0) = \frac{1}{[4\pi D(t - t_0)]^{3/2}} \exp \left[ \frac{(\mathbf{R} - \mathbf{R}_0)^2}{4D(t - t_0)} \right]$$  \hspace{1cm} \text{(Solution)}$$

$p^R (\mathbf{R}, t \mid \mathbf{R}_0, t_0)$: probability distribution of the vector $\mathbf{R}$ at time $t$, given that it was located at position $\mathbf{R}_0$ at time $t_0$

$D = D_A + D_B$: Sum of the diffusion coefficients

Free diffusive motion* of the inter-particle separation vector \( r \)

\[
\frac{\partial p^r(r, t | r_0, t_0)}{\partial t} = D \nabla_r^2 p^r(r, t | r_0, t_0) \quad \text{(DE)}
\]

\[
p^r(r, t | r_0, t_0) = \delta(r - r_0) \quad \text{(Initial condition)}
\]

For chemical reactions, we need the inter-particle distance \( r \).
- Therefore, the DE is written in spherical coordinates.
- Only the radial component will be considered (angular dependency terms are neglected). This considerably simplifies the analytical solution.

\[
\frac{\partial p(r, t | r_0)}{\partial t} = \frac{D}{r^2} \frac{\partial}{\partial r} \left[ r^2 \frac{\partial}{\partial r} p(r, t | r_0) \right] \quad \text{(Radial part of the DE)}
\]

\[
4\pi r_0^2 p(r, t | r_0) = \delta(r - r_0), \quad r \geq R \quad \text{(Initial condition; } R=\text{reaction radius)}
\]

\[ p(r, t | r_0, t_0) : \text{probability distribution of the separation distance } r \text{ at time } t, \text{ given that it was } r_0 \text{ at time } t_0 \]

*We assume that there is no force interacting between particles. This is the case for most of the chemical reactions that we are interested in.
Bimolecular reactions

Simple case: reaction with rate $k_a$

\[ A + B \rightarrow C \]

\[ \frac{4\pi R^2 D}{D} \frac{\partial p(r, t | r_0)}{\partial r} \bigg|_{r=R} = k_a p(R, t | r_0) \]

\[ 4\pi r_0 p(r, t | r_0) = \frac{1}{\sqrt{4\pi Dt}} \left\{ \exp \left[ -\frac{(r - r_0)^2}{4Dt} \right] + \exp \left[ -\frac{(r + r_0 - 2R)^2}{4Dt} \right] \right\} + \alpha W \left( \frac{r + r_0 - 2R}{\sqrt{4Dt}}, -\alpha \sqrt{Dt} \right) \]

\[ Q(t | r_0) = \int_{r}^{\infty} 4\pi r^2 p(r, t | r_0) dr = 1 + \frac{R\alpha + 1}{r_0\alpha} W \left( \frac{r_0 - R}{\sqrt{4Dt}}, \alpha \sqrt{Dt} \right) - \text{Erfc} \left( \frac{r_0 - R}{\sqrt{4Dt}} \right) \]

\[ \alpha = -\frac{k_a + 4\pi RD}{4\pi R^2 D} \]

The probability of reaction $P(t|r_0) = 1 - Q(t|r_0)$. At each time step, the probability of reaction is assessed. If the particles have not reacted, their relative distance is obtained by sampling the Green’s function.

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Green’s function for radiation chemistry

- Partially diffusion-controlled ABC reaction

\[ \frac{\partial p(r, t | r_0)}{\partial t} = \frac{D}{r^2} \frac{\partial}{\partial r} \left[ r^2 \frac{\partial}{\partial r} p(r, t | r_0) \right] \]

Diffusion equation (radial)

\[ 4\pi r_0^2 p(r, t | r_0) = \delta(r - r_0) \]

Initial condition

\[ 4\pi r_0 p(r, t | r_0) = \frac{1}{\sqrt{4\pi Dt}} \left[ \exp \left( -\frac{(r - r_0)^2}{4Dt} \right) + \exp \left( -\frac{(r + r_0 - 2R)^2}{4Dt} \right) \right] + \alpha(\beta + \alpha)(\gamma + \alpha) W \left( \frac{r + r_0 - 2R}{\sqrt{4Dt}}, -\alpha \sqrt{Dt} \right) + \frac{\beta(\gamma + \beta)(\alpha + \beta)}{(\gamma - \beta)(\alpha - \beta)} W \left( \frac{r + r_0 - 2R}{\sqrt{4Dt}}, -\beta \sqrt{Dt} \right) \]

Green’s function

\[ \alpha + \beta + \gamma = -(1 + k_a / k_d) / R \]

\[ \alpha\beta + \beta\gamma + \gamma\alpha = (k_e + k_d) / D \]

Coefficients

\[ \alpha\beta\gamma = -[(1 + k_a / k_d)k_e + k_d] / DR \]

System

\[ k_a, k_d \text{ and } k_e: \text{ reaction rate constants} \]
Green’s functions for radiation chemistry

- Partially diffusion-controlled reversible ABC reaction

  - Time discretization equations for \( p(r,t|r_0) \) and \( p(*,t|r_0) \)

\[
p(r, \Delta t_1 + \Delta t_2 \mid r_0) = \int_R^{\infty} 4\pi r^2 p(r, \Delta t_2 \mid r_1)p(r_1, \Delta t_1 \mid r_0)dr_1 + p(r, \Delta t_2 \mid *)p(*, \Delta t_1 \mid r_0)
\]

\[
p(*, \Delta t_1 + \Delta t_2 \mid r_0) = \int_R^{\infty} 4\pi r^2 p(*, \Delta t_2 \mid r_1)p(r_1, \Delta t_1 \mid r_0)dr_1 + p(*, \Delta t_2 \mid *)p(*, \Delta t_1 \mid r_0)
\]

  - Time discretization equations for \( p(r,t|*) \) and \( p(*,t|*) \)

\[
p(r, \Delta t_1 + \Delta t_2 \mid *) = \int_R^{\infty} 4\pi r^2 p(r, \Delta t_2 \mid r_1)p(r_1, \Delta t_1 \mid *)dr_1 + p(r, \Delta t_2 \mid *)p(*, \Delta t_1 \mid *)
\]

\[
p(*, \Delta t_1 + \Delta t_2 \mid *) = \int_R^{\infty} 4\pi r^2 p(*, \Delta t_2 \mid r_1)p(r_1, \Delta t_1 \mid *)dr_1 + p(*, \Delta t_2 \mid *)p(*, \Delta t_1 \mid *)
\]

- Proven numerically in Mathematica for all tested values of the parameters

Green’s function for radiation chemistry

\[
\begin{align*}
&k_a \quad k_c \\
&A + B \xrightarrow{\leftarrow} C \rightarrow \text{Products} \\
&k_d
\end{align*}
\]

Green’s functions

Survival and binding probabilities

Green’s functions for radiation chemistry

- Partially diffusion-controlled ABCD reaction
  \[4\pi a_i^2 D_i \frac{\partial p_i(x, t | x_0)}{\partial x_i} \bigg|_{x_i=x_0} = k_1 p_1(a_1, t | x_0) - k_2 p_2(a_2, t | x_0)\]

  \[p_i(x, t | x_0) = p_{ref_i}(x, t | x_0) - \frac{k_i a_i^2}{\sqrt{\tau_1 \tau_2} k_{D_i} x_0} \left[ \frac{\sigma_+}{\sigma_+ - \sigma_-} \frac{1 - \sigma_+ \sqrt{\tau_2}}{1 - \sigma_+ \sqrt{\tau_1}} W(\chi_1, \chi_0, \sigma_+ \sqrt{t}) \right. \]
  \[- \left. \frac{\sigma_-}{\sigma_+ - \sigma_-} \frac{1 - \sigma_- \sqrt{\tau_2}}{1 - \sigma_- \sqrt{\tau_1}} W(\chi_1, \chi_0, \sigma_- \sqrt{t}) \right]

  \[p_{ref_i}(x, t | x_0) = \frac{1}{4\pi x_0 a_i} \left[ \sqrt{\frac{\tau_1}{4\pi}} \left( e^{-(\chi_1 - \chi_0)^2} + e^{-(\chi_1 + \chi_0)^2} \right) - W(\chi_1, \chi_0, \frac{t}{\tau_1}) \right] \]

  \[p_2(y, t | x_0) = \frac{k_1 a_1 a_2}{\sqrt{\tau_1 \tau_2} k_{D_1} k_{D_2} y_0} \left[ \sigma_+ W(\chi_0 + \gamma_1, \sigma_+ \sqrt{t}) - \sigma_+ W(\chi_0 + \gamma_1, \sigma_- \sqrt{t}) \right] \]

  \[p_{AB\rightarrow CD}(t | x_0) = \frac{a_i}{x_0} \left( \frac{k_i}{k_{D_i}} \right) \left( \frac{1}{1 + k_i/k_{D_i} + k_i/k_{D_i}} \right) \left[ \text{Erf} \chi_0 + \frac{\sigma_-}{\sigma_+ - \sigma_-} \frac{(1 - \sigma_- \sqrt{\tau_2})}{(1 - \sigma_+ \sqrt{\tau_2})} W(\chi_0, \sigma_- \sqrt{t}) - \frac{\sigma_-}{\sigma_+ - \sigma_-} W(\chi_0, \sigma_+ \sqrt{t}) \right] \]

  \[\sigma_\pm = \frac{1}{2} \left[ \mu_1 + \mu_2 \pm \sqrt{(\mu_1 - \mu_2)^2 + \lambda} \right] \]
  \[\mu_1 = (1 + k_i/k_{D_i})/\sqrt{\tau_i} \]
  \[\mu_2 = (1 + k_i/k_{D_i})/\sqrt{\tau_i} \]
  \[\lambda = \frac{4k_1 k_2}{k_{D_1} k_{D_2} \sqrt{\tau_1 \tau_2}} \]

Boundary conditions

Green’s function \(x_0 \rightarrow x_1\) (AB→AB)

Green’s function \(x_0 \rightarrow y_1\) (AB→CD)

Probability of reaction AB→CD

- Boundary conditions

Green’s functions for radiation chemistry

- Partially diffusion-controlled reversible ABCD reaction
  - Time discretization equations for $p_1$ and $p_2$
    
    $p_1(x_2, t_1 + t_2 \mid x_0) = \int_{a_1}^{\infty} p_1(x_2, t_1 \mid x_1)p_1(x_1, t_1 \mid x_0)4\pi x_1^2 dx_1 + \int_{a_2}^{\infty} p_4(x_2, t_1 \mid y_1)p_2(y_1, t_1 \mid x_0)4\pi y_1^2 dy_1$

    $p_2(y_2, t_1 + t_2 \mid x_0) = \int_{a_1}^{\infty} p_2(y_2, t_1 \mid x_1)p_1(x_1, t_1 \mid x_0)4\pi x_1^2 dx_1 + \int_{a_2}^{\infty} p_3(y_2, t_1 \mid y_1)p_2(y_1, t_1 \mid x_0)4\pi y_1^2 dy_1$

  - Time discretization equations for $P_{AB\rightarrow CD}$

    $P_{AB\rightarrow CD}(t_1 + t_2 \mid x_0) = \int_{a_1}^{\infty} P_{AB\rightarrow CD}(t_2 \mid x_1)p_1(x_1, t_1 \mid x_0)4\pi x_1^2 dx_1 + \int_{a_2}^{\infty} (1 - P_{CD\rightarrow AB}(t_2 \mid y_1))p_2(y_1, t_1 \mid x_0)4\pi y_1^2 dy_1$

- Similar equations for $p_3, p_4$ and $P_{CD\rightarrow AB}$
- Proven numerically in Mathematica for all tested values of the parameters

Green’s functions for radiation chemistry

\[ A + B \xleftrightarrow{k_1, k_2} C + D \]

Green’s functions

Survival and binding probabilities

Radiation chemistry

See video at: http://youtu.be/If29Rs4fDO4
Primary yields of $e_{aq}^-$, OH, H, H$_2$ and H$_2$O$_2$ as a function of the LET

Irradiation by 300-0.1 MeV protons
LET: ~0.3-85 keV/μm

Note: the primary yields (noted $G_X$) are the yields at the end of spur expansion ($\sim 10^{-6}$ s)

The radiation chemistry of DNA is very complex.

Many reaction rate constants are known.

<table>
<thead>
<tr>
<th>Reaction</th>
<th>$k$ (dm$^3$.mol$^{-1}$.s$^{-1}$)</th>
<th>Radius (Å)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$e^{-}_{aq} + \text{Thymine} \rightarrow \text{Thy}(+e)$</td>
<td>$1.79 \times 10^{10}$</td>
<td>5.287</td>
</tr>
<tr>
<td>$\cdot \text{OH} + \text{Thymine} \rightarrow \text{TC5OH} + \text{TC6OH} + \text{TUCH2}^-$</td>
<td>$6.4 \times 10^{9}$</td>
<td>3.02</td>
</tr>
<tr>
<td>$\text{H.} + \text{Thymine} \rightarrow \text{Thymine}^*$</td>
<td>$5.7 \times 10^{8}$</td>
<td>0.11</td>
</tr>
</tbody>
</table>
The software RITRACKS

- The software RITRACKS comprises several parts
  - The calculation part includes:
    - The cross sections, which are necessary for particle transport
    - The particle transport routines
    - Post-simulation data management
  - The Graphic User Interface (GUI), comprises several windows:
    - The main window
    - Incident radiation window
    - Multi-CPU support
    - Cross sections windows (electrons and ions)
    - Results (events) details
  - The 3D visualization window
  - The help file

- All necessary files are included in an installer for Windows
Using RITRACKS

- The installer
  - The necessary files are included in an installer created by the freeware InstallJammer
  - The program is installed in the folder C:\Program Files (x86)\RITRACKS
  - Simulations are stored in the subfolder RITRACKS Simulations in the My Documents folder
### RITRACKS main window

#### Incident radiation
- **Electron**
- **Ion**: 12C6+

#### Irradiation volume
- **Disk**
- **Square**

- **No particles**: 1
- **Radius**: 0 um
- **Length**: 5 um

#### Simulation info
- **Histories**: 10

#### Calculations
- **Save track structure**
- **Save all events**
- **Save 3D-dose map**

#### Messages
- Welcome to RITRACKS

#### Buttons
- **Start simulation**
- **3D tracks**
- **Simulation progress**: 
- **Results details**

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The following information is given in this window

Rest mass energy: \( M c^2 \)

Total energy: \( \gamma M c^2 \)

Relativistic \( \gamma \): \( \gamma = \frac{T}{M c^2} + 1 \)

Relativistic \( \beta \): \( \beta^2 = 1 - \frac{1}{\gamma^2} \)

Momentum: \( p = \gamma M v \)

Maximum energy transfer to e\(^-\): \( E_{\text{max}} = \frac{2mc^2(\gamma^2 - 1)}{1 + 2\gamma(m/M) + (m/M)^2} \)

\( \gamma \):
- Kinetic energy: 25 MeV/amu
- Rest mass energy: 11258.939814 MeV
- Total energy: 11558.940988 MeV
- \( \beta^2 \): 0.051234
- \( \beta \): 0.22635
- \( \gamma \): 1.026646
- \( p \): 2616.36982 MeV/c
- \( Q_{\text{max}} \): 55.127 keV
- \( Z_{\text{eff}} \): 6
- LET (appr): 78.27 keV/um

LET (MeV/cm): 
\[ \frac{dE}{dx} = \frac{0.170}{\beta^2} \left[ F(\beta) - 4.31 \right] \]

\( F(\beta) = \ln \frac{1.02 \times 10^6 \beta^2}{1 - \beta^2} - \beta^2 \)
Electron cross sections window

![Electron cross sections window](image)
Visualization window

Tools:
- Rotation
- Translation
- Zoom
- Save to file
- Copy to clipboard
- Create a .avi file
- Open data folder

Visualization:
- Radiolytic species
- Events
- Dose (voxels)

Time evolution
RITRACKS tools

- Calculation of tracks per cell in a cell culture for a given ion, energy and dose
Release history

- RITRACKS was used by the students at the NASA Space Radiation Summer School at the Brookhaven National Laboratory, Upton, New York (June 6-24, 2011, May 28 - June 15, 2012, MIT ICED June 2012) (over 40 users)
- The release to international partners was approved in 2011
- RITRACKS was released to NASA space radiation community with over 20 users
- The software is now available for download on the web site http://spaceradiation.usra.edu/irModels (ITAR, authentication and password required)

http://spaceradiation.usra.edu
Release history

- An online version of RITRACKS will be available soon!

Left: Simulation of a $^{12}$C$^{6+}$, 60 MeV/amu, on the projected RRAW site.

Right: Calculation of the radial dose for the track depicted on the left.

The track structure data and the radial dose are available for download after calculation.
Future plans for development and use

- Android/iPhone version

- For ions:
  - LET
  - Relativistic β and γ
  - $Z_{\text{eff}}$ and $Z_{\text{eff}}^{2/\beta^2}$
  - Maximum energy transfer to an electron
  - Dose and fluence
  - Radial dose
  - Number of hits per cell
  - in a cell culture

- For electrons:
  - Relativistic β and γ
  - Range

![RITRACKS screenshot showing calculations for 12C6+ ion with energy of 290 MeV/u, cell area of 7.8e-7 cm², and dose of 0.1 Gy. The average tracks per cell is calculated to be 3.78.](image)
Future plans for development and use

- Implementation of the non-homogeneous chemistry
- Predictions of clustered and complex DNA damage yields in human cells for improving the understanding of DNA repair and signal transduction
- Use with chromosome models to study double-strand breaks (DSB) in relation to cancer risks from space radiation
- Web-based version
- New GPU-CPU version to improve computational speeds by several orders of magnitude.
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- Dr. Francis Cucinotta (UNLV)
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- Radiation Biophysics group at JSC
- USRA
- NASA
References

The software RITRACKS

- Multiple CPU computing (Windows)

RITRACKS V3

Select the CPUs you want to use

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