

# Supplementary Materials: TRAX-CHEMxt: Towards the Homogeneous Chemical Stage of Radiation Damage

Gianmarco Camazzola, Daria Boscolo, Emanuele Scifoni, Alexander Dorn, Marco Durante, Michael Krämer, Valentino Abram and Martina C. Fuss

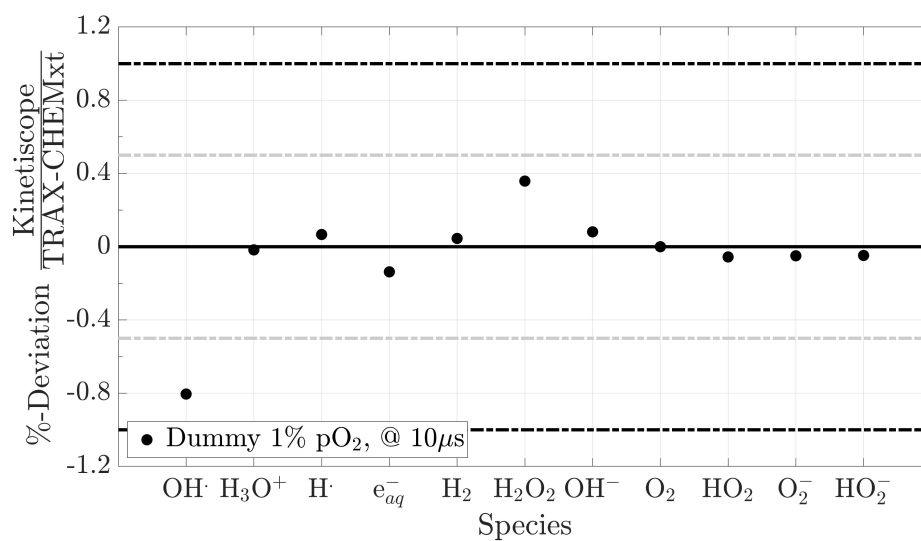
**Table S1.** List of reactions, respective reaction rate constants and diffusion coefficients implemented in TRAX-CHEMxt, identical to the ones simulated in TRAX-CHEM. The  $\kappa$  values are determined under normal conditions, i.e. neutral pH and 25 °C. Adapted from [1].

	Reaction	$\kappa$ ( $10^{10} \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ )
(i)	$\text{OH}^\bullet + \text{OH}^\bullet \rightarrow \text{H}_2\text{O}_2$	0.6
(ii)	$\text{OH}^\bullet + \text{e}_{\text{aq}}^- \rightarrow \text{OH}^-$	2.2
(iii)	$\text{OH}^\bullet + \text{H}^\bullet \rightarrow \text{H}_2\text{O}$	2.0
(iv)	$\text{OH}^\bullet + \text{H}_2 \rightarrow \text{H}^\bullet + \text{H}_2\text{O}$	0.0045
(v)	$\text{OH}^\bullet + \text{H}_2\text{O}_2 \rightarrow \text{HO}_2^\bullet + \text{H}_2\text{O}$	0.0023
(vi)	$\text{e}_{\text{aq}}^- + \text{e}_{\text{aq}}^- + \text{H}_2\text{O} + \text{H}_2\text{O} \rightarrow \text{H}_2 + \text{OH}^- + \text{OH}^-$	0.55
(vii)	$\text{e}_{\text{aq}}^- + \text{H}^\bullet + \text{H}_2\text{O} \rightarrow \text{H}_2 + \text{OH}^-$	2.5
(viii)	$\text{e}_{\text{aq}}^- + \text{H}_3\text{O}^+ \rightarrow \text{H}^\bullet + \text{H}_2\text{O}$	1.7
(ix)	$\text{e}_{\text{aq}}^- + \text{H}_2\text{O}_2 \rightarrow \text{OH}^\bullet + \text{OH}^-$	1.0
(x)	$\text{H}^\bullet + \text{H}^\bullet \rightarrow \text{H}_2$	1.0
(xi)	$\text{H}^\bullet + \text{H}_2\text{O}_2 \rightarrow \text{OH}^\bullet + \text{H}_2\text{O}$	0.01
(xii)	$\text{H}^\bullet + \text{OH}^- \rightarrow \text{e}_{\text{aq}}^- + \text{H}_2\text{O}$	0.002
(xiii)	$\text{H}_3\text{O}^+ + \text{OH}^- \rightarrow \text{H}_2\text{O} + \text{H}_2\text{O}$	10.0
(xiv)	$\text{e}_{\text{aq}}^- + \text{O}_2 \rightarrow \text{O}_2^{\bullet -}$	1.9
(xv)	$\text{H}^\bullet + \text{O}_2 \rightarrow \text{HO}_2^\bullet$	2.0
(xvi)	$\text{OH}^\bullet + \text{HO}_2^\bullet \rightarrow \text{O}_2 + \text{H}_2\text{O}$	1.0
(xvii)	$\text{OH}^\bullet + \text{O}_2^{\bullet -} \rightarrow \text{O}_2 + \text{OH}^-$	0.9
(xviii)	$\text{OH}^\bullet + \text{HO}_2^- \rightarrow \text{HO}_2^\bullet + \text{OH}^-$	0.5
(xix)	$\text{e}_{\text{aq}}^- + \text{HO}_2^\bullet \rightarrow \text{HO}_2^-$	2.0
(xx)	$\text{e}_{\text{aq}}^- + \text{O}_2^{\bullet -} + \text{H}_2\text{O} \rightarrow \text{OH}^- + \text{HO}_2^-$	1.3
(xxi)	$\text{H}^\bullet + \text{HO}_2^\bullet \rightarrow \text{H}_2\text{O}_2$	2.0
(xxii)	$\text{H}^\bullet + \text{O}_2^{\bullet -} \rightarrow \text{HO}_2^-$	2.0
(xxiii)	$\text{H}_3\text{O}^+ + \text{O}_2^{\bullet -} \rightarrow \text{HO}_2^\bullet + \text{H}_2\text{O}$	3.0
(xxiv)	$\text{H}_3\text{O}^+ + \text{HO}_2^- \rightarrow \text{H}_2\text{O}_2 + \text{H}_2\text{O}$	2.0
(xxv)	$\text{HO}_2^\bullet + \text{HO}_2^\bullet \rightarrow \text{H}_2\text{O}_2 + \text{O}_2$	0.000076
(xxvi)	$\text{HO}_2^\bullet + \text{O}_2^{\bullet -} \rightarrow \text{O}_2 + \text{HO}_2^-$	0.0085

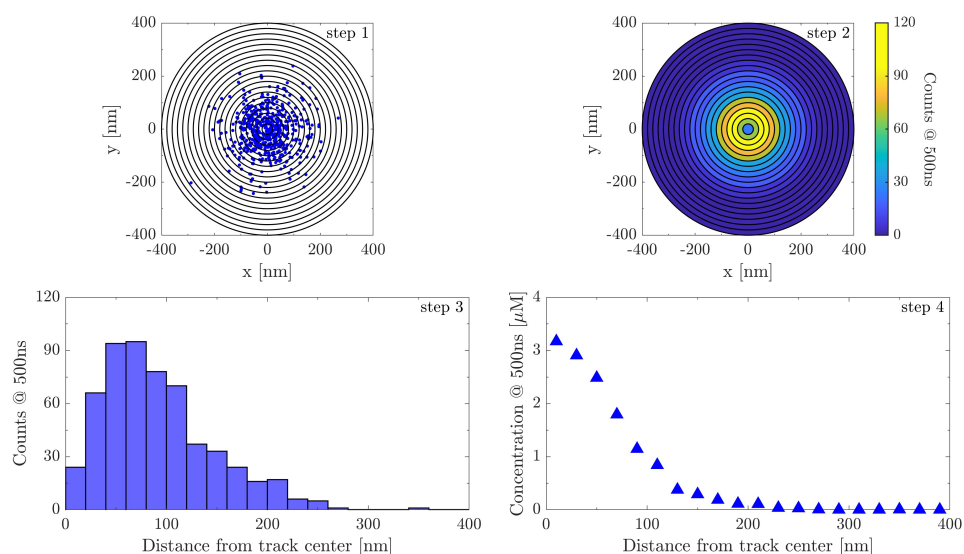
Species	$D$ ( $10^{-9} \text{ m}^2 \text{ s}^{-1}$ )
$\text{OH}^\bullet$	2.8
$\text{H}_3\text{O}^+$	9.0
$\text{H}^\bullet$	7.0
$\text{e}_{\text{aq}}^-$	4.5
$\text{H}_2$	4.8
$\text{H}_2\text{O}_2$	2.3
$\text{OH}^-$	5.0
$\text{O}_2$	2.1
$\text{HO}_2^\bullet$	2.0
$\text{O}_2^{\bullet -}$	2.1
$\text{HO}_2^-$	2.0

**Table S2.** Deviations associated with TRAX-CHEMxt, for all the initial conditions simulated so far. Each deviation is derived by taking the biggest value from the differences between the total number of every radical and molecule predicted by the extension (with initial concentrations taken at 600 ns) and the respective quantities produced by TRAX-CHEM, divided by the latter. To determine these values, the contributions from  $\text{HO}_2^-$  have been disregarded due to their very low yields.

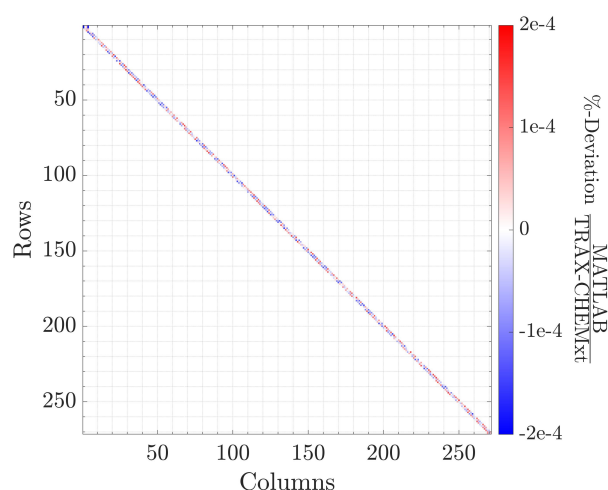
Particle type	Energy	pO <sub>2</sub> (atm)	Deviation at 1 $\mu\text{s}$
Electrons	500 keV	0%	1%
Electrons	500 keV	0.5%	1%
Electrons	500 keV	1%	1%
Electrons	500 keV	3%	1%
Electrons	500 keV	7%	1%
Electrons	500 keV	21%	2%
Electrons	1 MeV	0%	1%
Protons	40 MeV	0%	1%
Protons	65 MeV	21%	2%
Protons	90 MeV	0%	1%
Protons	90 MeV	4%	1%
Protons	90 MeV	21%	2%
Helium ions	150 MeV/u	21%	2%
Carbon ions	10 MeV/u	21%	6%
Carbon ions	20 MeV/u	21%	6%
Carbon ions	40 MeV/u	0%	4%
Carbon ions	40 MeV/u	3%	5%
Carbon ions	40 MeV/u	21%	5%
Carbon ions	90 MeV/u	0%	4%
Carbon ions	90 MeV/u	0.5%	4%
Carbon ions	90 MeV/u	2%	4%
Carbon ions	90 MeV/u	3%	4%
Carbon ions	90 MeV/u	7%	5%
Carbon ions	90 MeV/u	21%	5%
Carbon ions	150 MeV/u	7%	4%
Carbon ions	300 MeV/u	21%	3%



**Figure S1.** Deviations between Kinetiscope and TRAX-CHEMxt, registered for a "dummy" case with uniform concentrations assigned randomly to each chemical species, in a water environment with  $pO_2 = 1\%$ . Marked with dash-dotted lines are discrepancies of  $\pm 0.5\%$  and  $\pm 1\%$ . Initial data handed over to both codes at  $1\ \mu s$ , and the chemical network in this reaction-limited domain was simulated up to  $10\ \mu s$ .



**Figure S2.** Steps constituting the conversion of the information from TRAX-CHEM to TRAX-CHEMxt. After collecting the positions of a specific radical or molecule around the track center (step 1) and counting its amount within each radial bin (step 2), the respective histogram is created (step 3). In conclusion, the various counts are converted into concentration values (step 4), supposing thus a uniform concentration within each radial bin. In the proposed example, a bin width and a transitional time of respectively  $20\ \text{nm}$  and  $500\ \text{ns}$  are used. The concentrations are assigned to the respective bin centers.



**Figure S3.** Deviations between the matrix values for the product  $M^{-1}N$ , computed by MATLAB and the implemented algorithm in TRAX-CHEMxt following [2], for the diffusion of the hydroxyl radical. The set of parameters exploited is: time step  $dt = 5 \cdot 10^{-10}$  s, diffusion coefficient  $D = 2.8 \cdot 10^9$  nm<sup>2</sup>/s, bin width (distance between two consecutive radii)  $bw \approx 20$  nm. The error is on the order of  $10^{-6}$ .

## References

1. Boscolo, D.; Krämer, M.; Fuss, M.C.; Durante, M.; Scifoni, E. Impact of target oxygenation on the chemical track evolution of ion and electron radiation. *Int. J. Mol. Sci.* **2020**, *21*, 424. <https://doi.org/10.3390/ijms21020424>.
2. Usmani, R.A. Inversion of Jacobi's tridiagonal matrix. *Comput. Math. Appl.* **1994**, *27*, 59–66. [https://doi.org/10.1016/0898-1221\(94\)90066-3](https://doi.org/10.1016/0898-1221(94)90066-3).

**Disclaimer/Publisher's Note:** The statements, opinions and data contained in all publications are solely those of the individual author(s) and contributor(s) and not of MDPI and/or the editor(s). MDPI and/or the editor(s) disclaim responsibility for any injury to people or property resulting from any ideas, methods, instructions or products referred to in the content.