An Extensible Reaction-Diffusion Solver for Radiolysis and Astroparticle Physics

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Theory of Water Radiolysis

[1] J.-P. Jay-Gerin, “Fundamentals of Water Radiolysis,” Encyclopedia, vol. 5, no. 1, p. 38, Mar. 2025, doi: 10.3390/encyclopedia5010038.

Pure Water Radiolysis

- The speciation scheme and mechanics of pure water radiolysis is well known.
- For a non-uniform radiation field, the chemistry stays inhomogeneous and macroscopic diffusion is relevant.
- In continuous irradiation, the stages occur simultaneously.

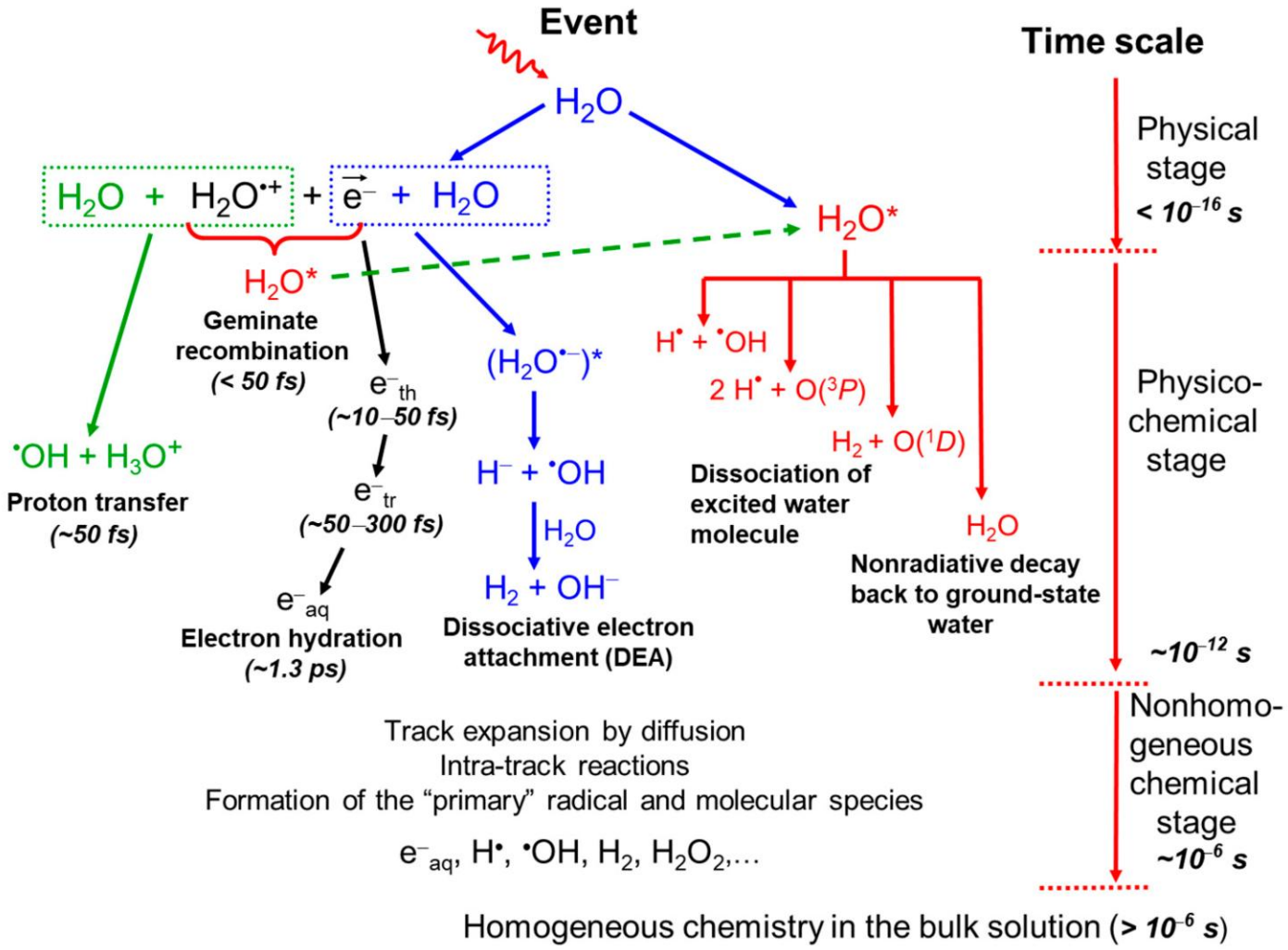


Diagram of stages of water radiolysis [1].

Theory of Water Radiolysis

Nitrogen in Water Radiolysis

- The speciation scheme is not well understood.
- A complex reaction network forms between water and diatomic nitrogen radiolysis products.

Experimental Research

- Susan Beale (MSc TRIUMF/SFU) is studying speciation in N_2-H_2-H_2O radiolysis systems.
- Primarily tracking NH_4^+ and NO_3^-.
- *How might N contribute to radiolysis and formation of more complex molecules → origins of life?*

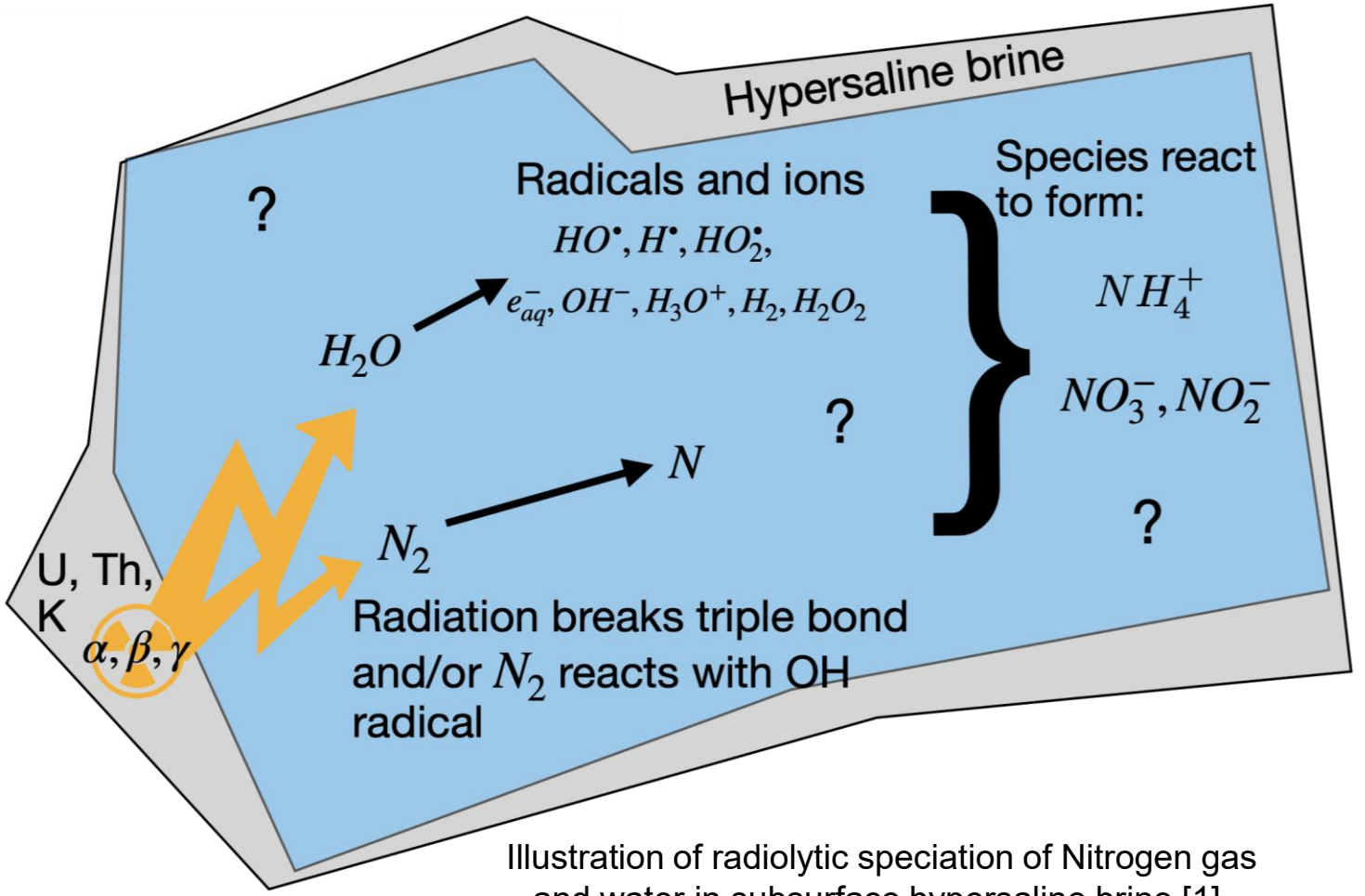


Illustration of radiolytic speciation of Nitrogen gas and water in subsurface hypersaline brine [1].

[1] S. Beale et al., "Investigations of Nitrogen Cycling in Ancient Subsurface Fluids." Goldschmidt, in-person Oral Presentation, Jul. 2026.

Mathematical Model

[1] E. Ibe et al., “Behavior of Nitrogen Compounds in Radiation Field and Nuclear Reactor Systems,” J. Nucl. Sci. Technol., 26, 760–769, 1989.

Radiolytic Source

The G value g_i is defined as the concentration change produced per unit of absorbed energy

Then, by definition, for H_2O primary radiolysis products,

$$G_i(t,x,u) = d(t,x)g_i$$

While for N_2 primary radiolysis products [1],

$$G_i(t,x,u) = 1.4d(t,x)g_i\frac{u_{\mathrm{N_2}}}{u_{\mathrm{H_2O}}}$$

Mass-Action Chemistry

For an elementary reaction

$$\sum_i a_i A_i \rightarrow \sum_i b_i B_i$$

The reaction rate is

$$r = -\frac{1}{a_i}\partial_t[A_i] = \frac{1}{b_i}\partial_t[B_i]$$

And by the law of mass-action,

$$r = k\prod_j [A_j]^{a_j}$$

So, for each radiolysis species,

$$K_i(u) = \sum_{j=1}^{M} a_{j,i}k_j \prod_{\ell=1}^{N} u_\ell^{a_\ell}$$

Macroscopic Diffusion

By Fick's Law, concentration flux at a point is

$$J = -D_i\nabla u_i(t,x)$$

Then concentration accumulating at a point is

$$-\nabla\cdot J = D_i\nabla^2 u_i(t,x).$$

u_i = species conc.,
d = dose-rate field,
$a_{j,i}$ = specie multiplicity in reaction,
k_j = reaction rate constant,
D_i = diffusion coeff.

Mathematical Model

Strong Form of Model PDE

Mass-Action Term + Radiolytic Source

$$R_i = K_i + G_i$$

Fickian Diffusion Term

Closed Container
(bounded Lipschitz domain)

$$\begin{cases} \partial_t u_i(t,x) = D_i \nabla^2 u_i(t,x) + R_i(t,x,u), & (t,x) \in (0,T] \times \Omega \\ \nabla u_i(t,x) \cdot n_{\partial\Omega}(x) = 0, & (t,x) \in (0,T] \times \partial\Omega \\ u_i(0,x) = I_i(x) \geq 0, & x \in \Omega \end{cases}$$

Neumann
Boundary Condition

Initial Concentration
Distribution

Model End Time

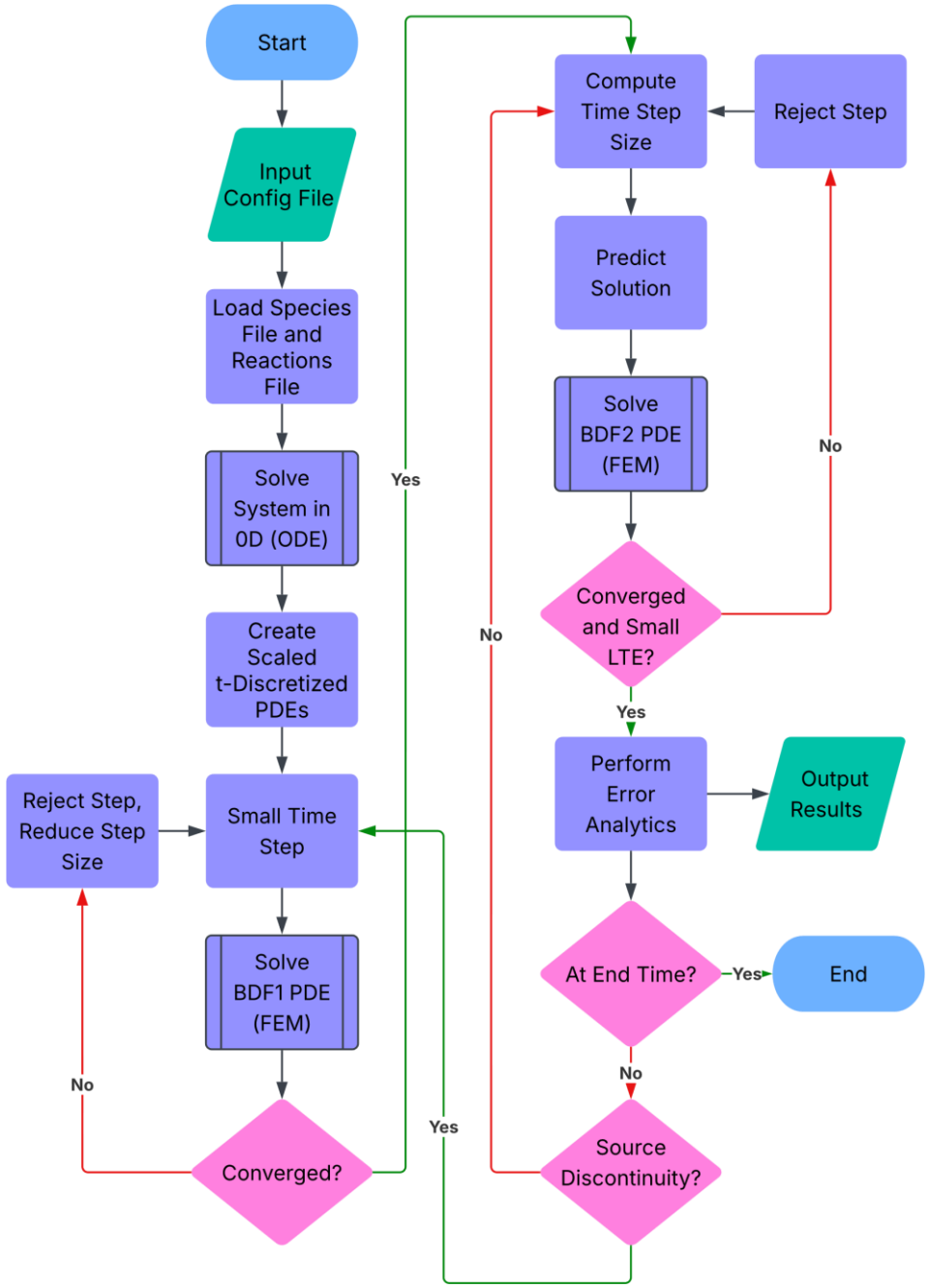
Solver Methods

Weak Form

The strong form of the model PDE is time-discretized using BDF1/BDF2 and then converted into the weak variational form.

Algorithm

The weak form is stepped over time using a quasi-constant step-size Nordsieck-type algorithm based on CVODE [1] and solved over space using finite element methods with FEniCSx [2].



Simplified solver algorithm flowchart

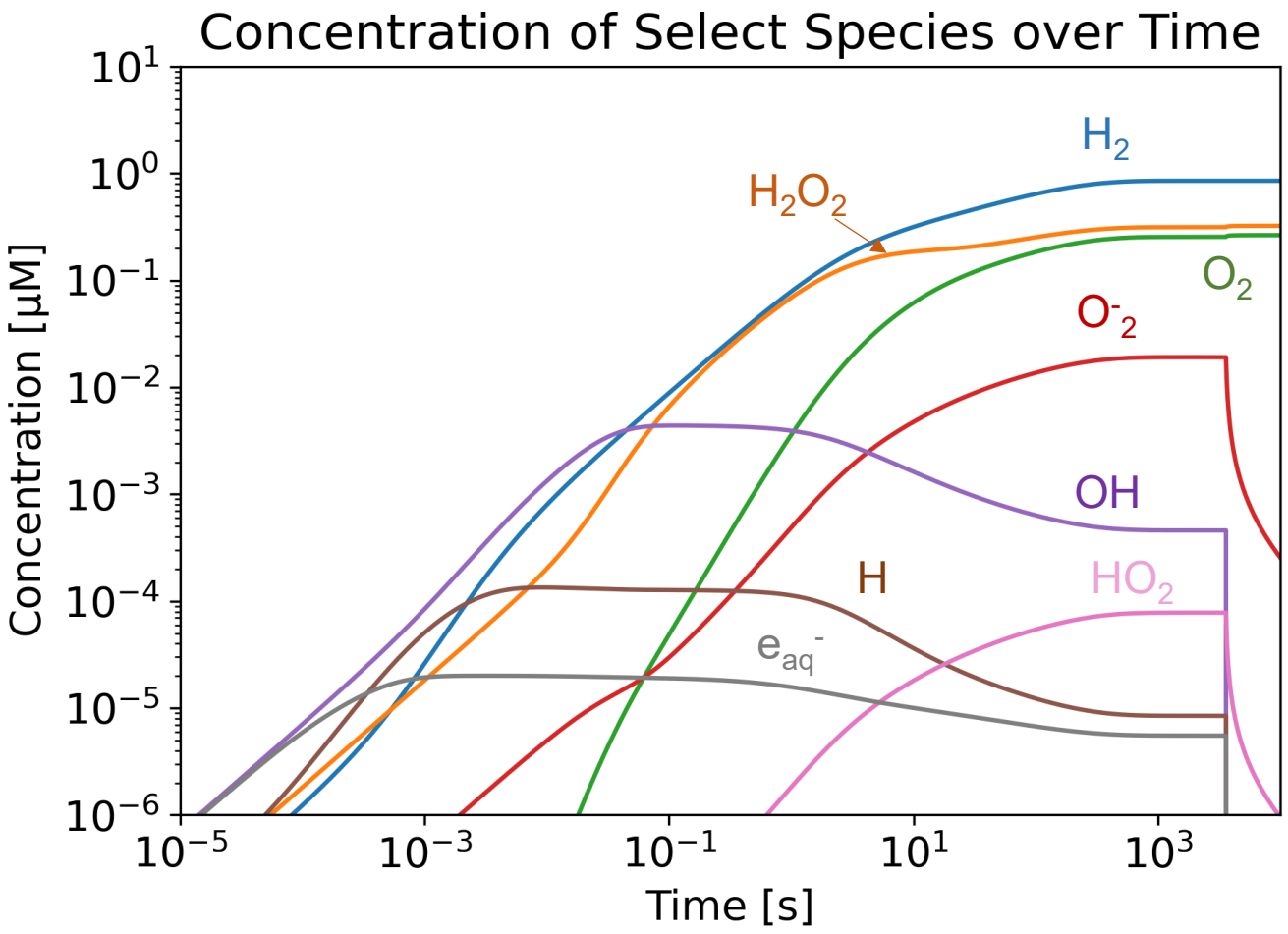
[1] A. C. Hindmarsh et al., “User Documentation for CVODE.” [Online].
[2] I. A. Baratta et al., “DOLFINx: The next generation FEniCS problem solving environment,” Dec. 2025.

[1] B. Pastina and J. A. LaVerne, “Effect of Molecular Hydrogen on Hydrogen Peroxide in Water Radiolysis,” J. Phys. Chem. A, 105, 9316–9322, 2001.

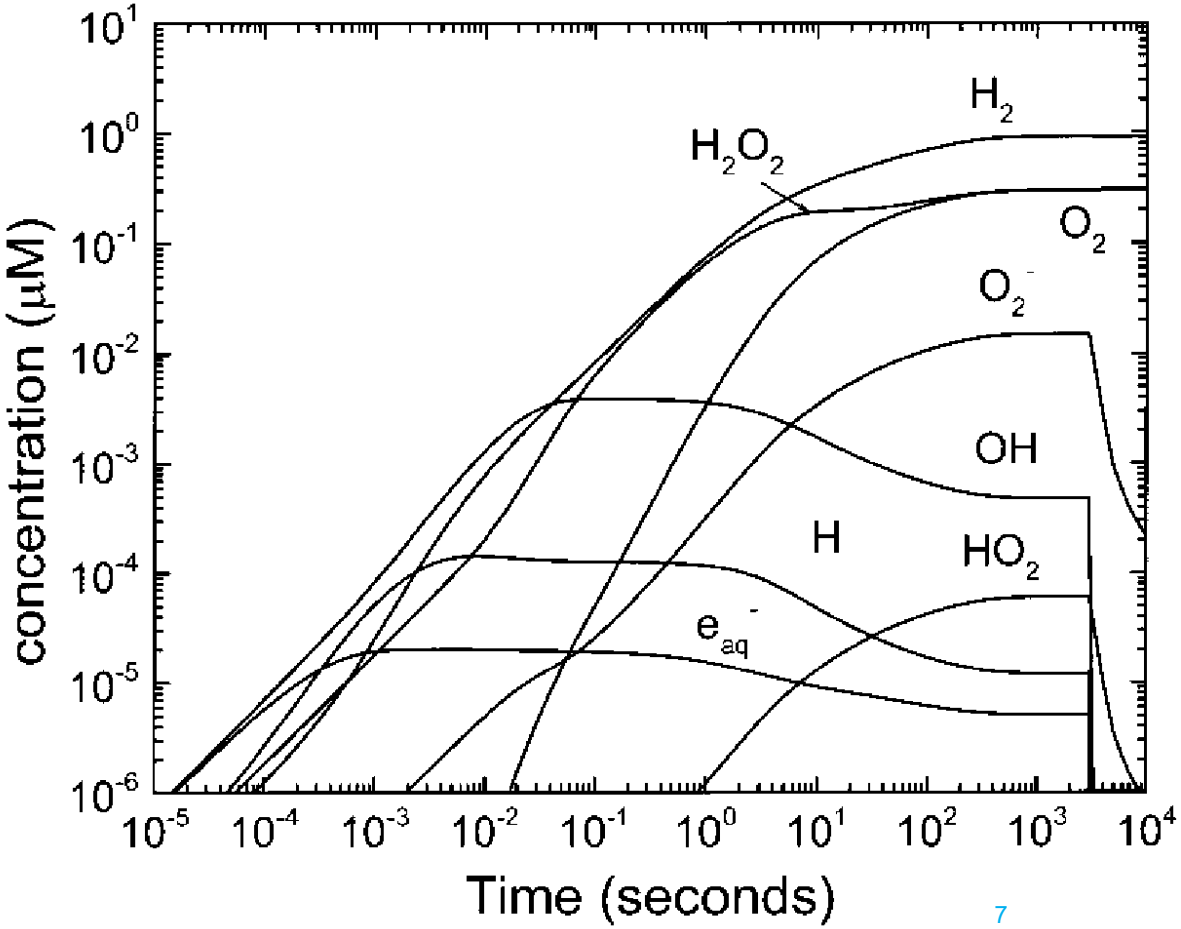
Results

Benchmarking: Homogeneous Water Radiolysis

Uniform 0.25Gy/s dose-rate field with initial concentrations, H_2O radiolysis G values, and reaction rate constants from Pastina et al. [1]. Dosing ends at 3.6×10^3s.



Reproduced Pastina’s radiolysis system



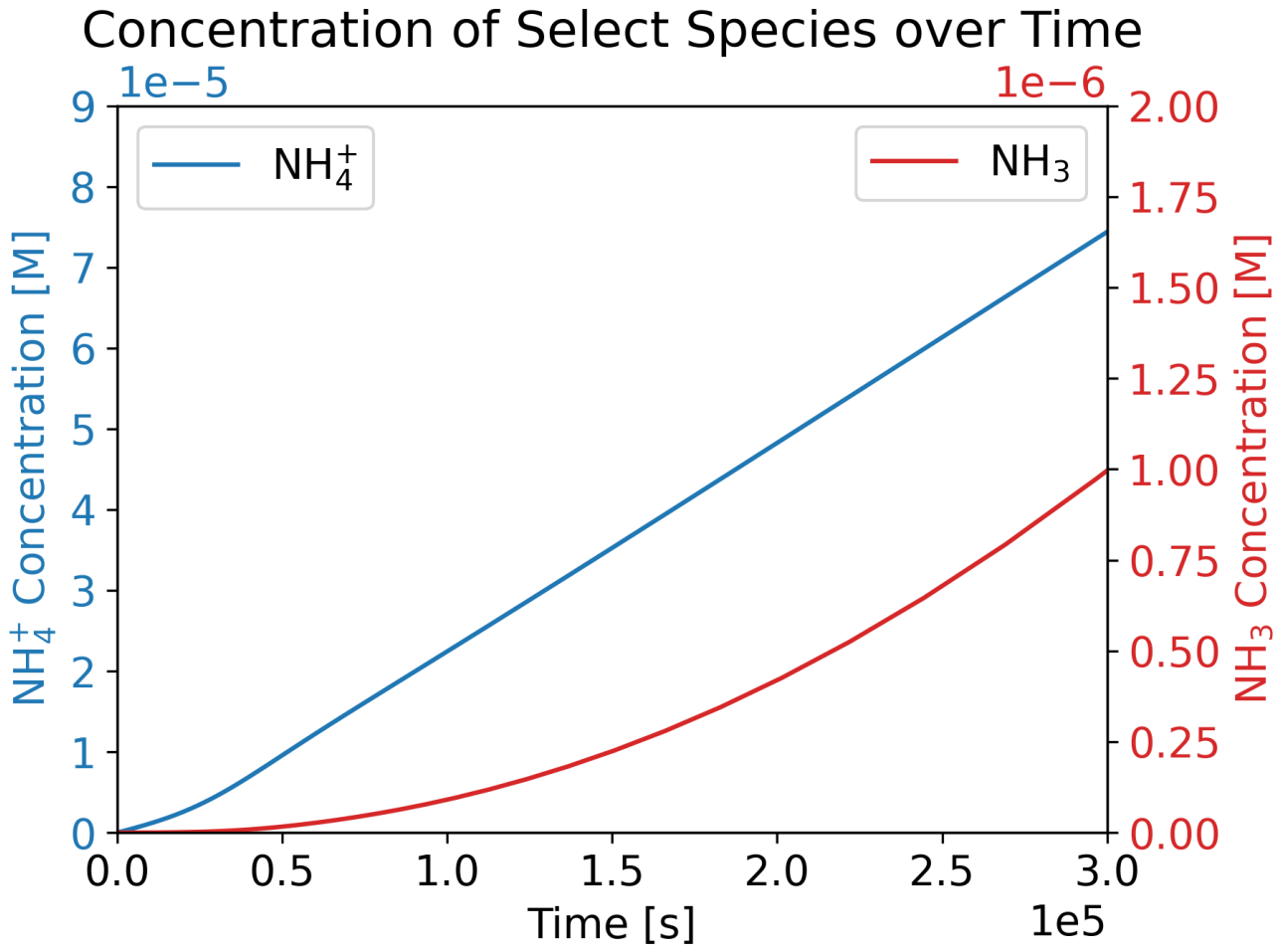
Pastina’s radiolysis system results

[1] E. Ibe et al., “Behavior of Nitrogen Compounds in Radiation Field and Nuclear Reactor Systems,” J. Nucl. Sci. Technol., 26, 760–769, 1989.

Results

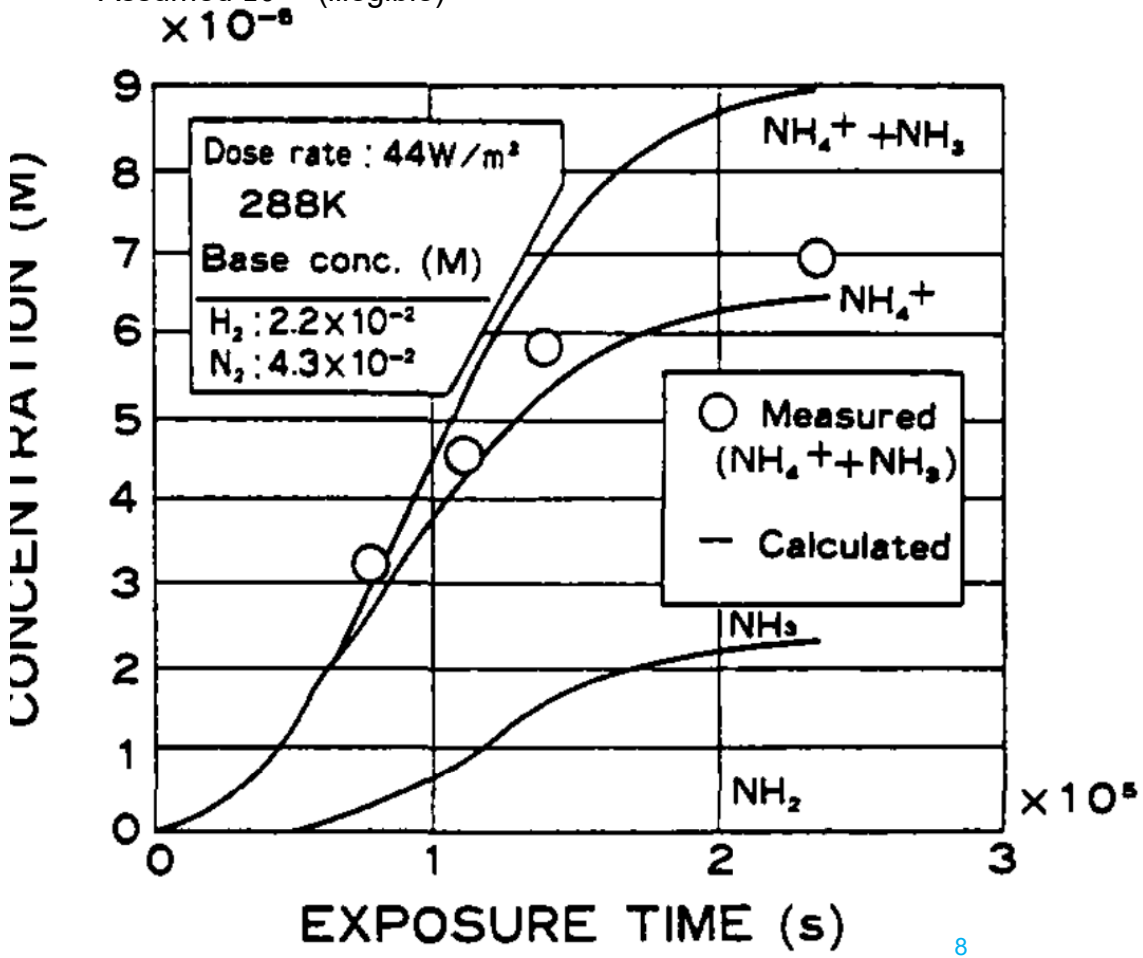
Benchmarking: Homogeneous Nitrogen and Water Radiolysis

Uniform 0.044Gy/s dose-rate field with initial concentrations, N_2-H_2-H_2O radiolysis G values, and reaction rate constants from Ibe et at. [1].



Reproduced Ibe’s radiolysis system

Assumed 10^{-5} (illegible)

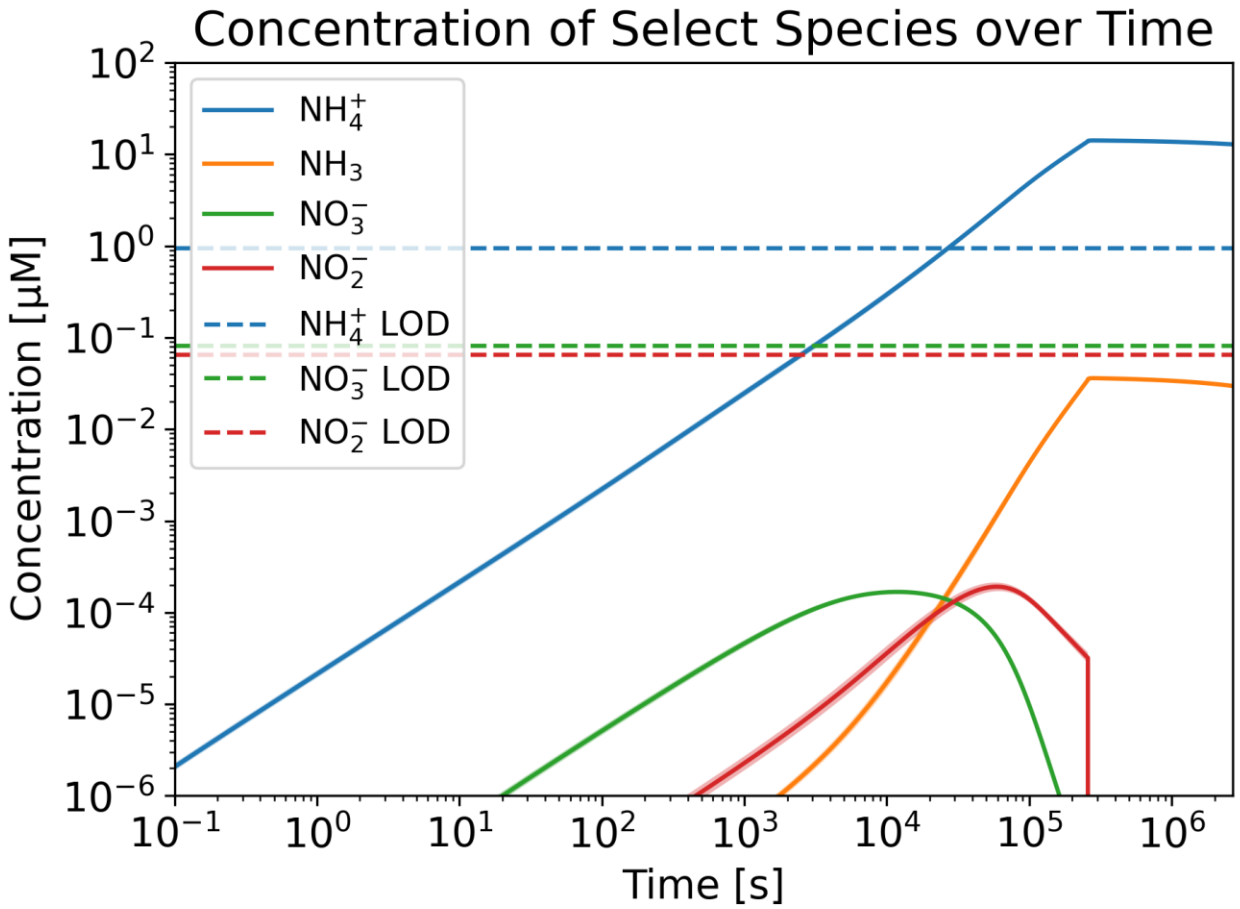


Ibe’s radiolysis system results

Results

Predicting: Nitrogen and Water Radiolysis Experiment

Attenuated 0.5Gy/s dose-rate field using initial conditions from Beale et al. [1], and N_2-H_2-H_2O radiolysis G values and reaction rate constants from Ibe et al. [2]. Dosing ends at 2.58×10^5s.



Simulated Beale's N_2-H_2-H_2O radiolysis system

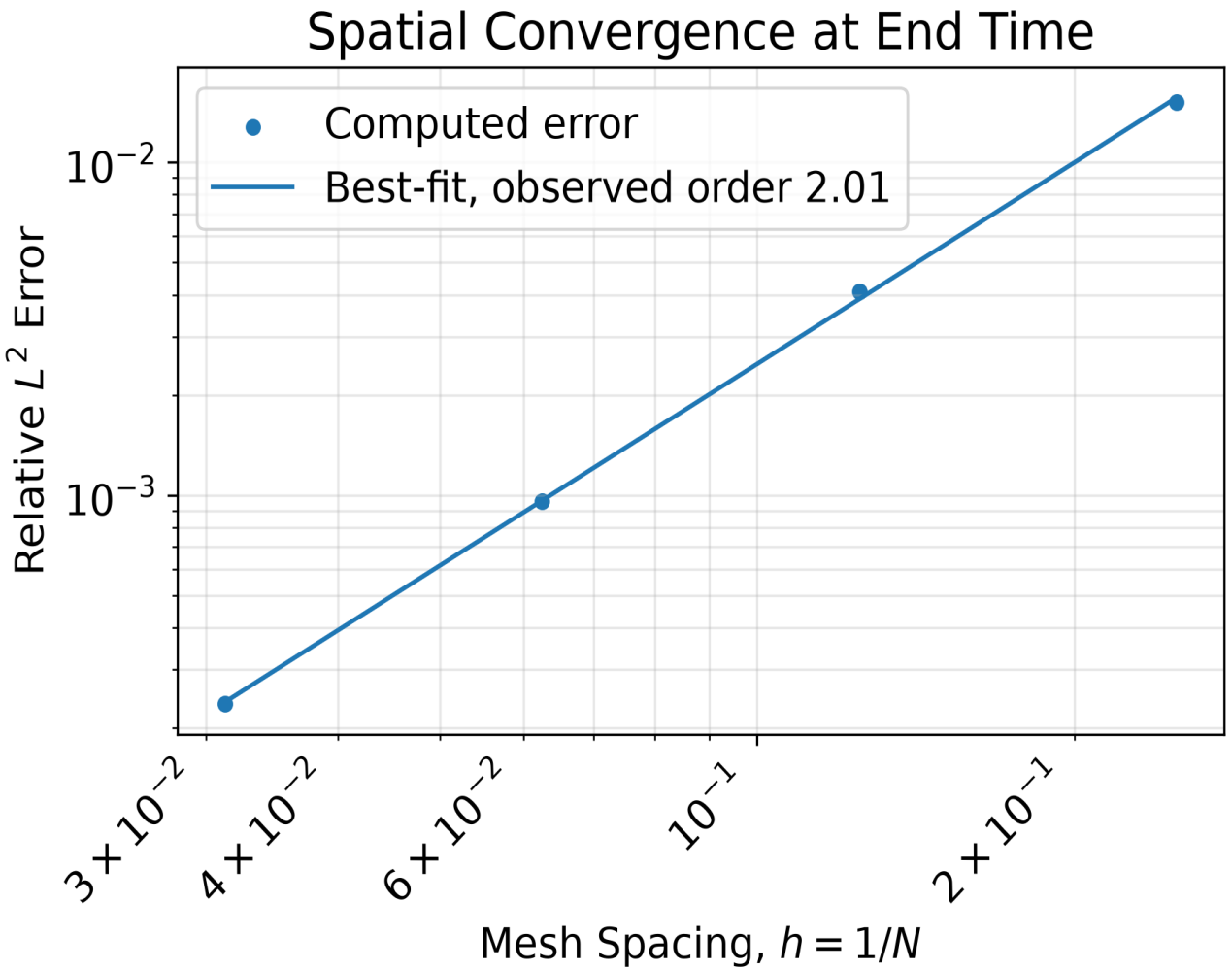
Species	Predicted Result	Beale et al. Result	Consistency
NH_4^+	Above LOD	Below LOD	Inconsistent
NO_3^-	Below LOD	Above LOD	Inconsistent
NO_2^-	Below LOD	Below LOD	Consistent

Why inconsistent?

1. Solver using reaction scheme by Ibe was already inconsistent.
2. The reaction scheme by Ibe is for a different model and physics regime.
3. Possible experimental error.

[1] S. Beale et al., "Investigations of Nitrogen Cycling in Ancient Subsurface Fluids." Goldschmidt, in-person Oral Presentation, Jul. 2026.
[2] E. Ibe et al., "Behavior of Nitrogen Compounds in Radiation Field and Nuclear Reactor Systems," J. Nucl. Sci. Technol., 26, 760–769, 1989.

Analysis



Spatial Discretization Error

- Spatial discretization order of accuracy was validated for Beale's system.
- Using Richardson's method from differences between successively refined meshes $N = 4 \rightarrow 64$.
- The observed order is consistent with the theoretical order of linear Lagrange elements being 2 under L^2.

Potential Future Applications

[1] S. Ekström, “Massive Star Modeling and Nucleosynthesis,” Front. Astron. Space Sci., vol. 8, Apr. 2021, doi: 10.3389/fspas.2021.617765.

This solver was built to be general-purpose and extensible in the realm of stiff source-driven reaction-diffusion systems.

Straightforward Applications

- H_2O_2 production in water-cooling pipes for TRIUMF’s beamline (investigating corrosion)
- Radiolytic chemistry in space (ex. chemistry on dust grains in molecular clouds).

Speculative Applications

- Stellar nucleosynthesis.
- Radiolysis in dark matter or neutrino detectors.
- Non-steady-state electroweak baryogenesis.
- And more… accepting suggestions!

Diffusion Term Reaction Term

$$\rho \frac{\mathrm{d}X_i}{\mathrm{d}t} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(\rho r^2 D \frac{\partial X_i}{\partial r}\right) + \left(\frac{\mathrm{d}X_i}{\mathrm{d}t}\right)_{\mathrm{nucl}}$$

Example stellar nucleosynthesis PDE [1]

Discussion

[1] E. Ibe et al., “Behavior of Nitrogen Compounds in Radiation Field and Nuclear Reactor Systems,” J. Nucl. Sci. Technol., 26, 760–769, 1989.

Unlikely Causes of Discrepancies

- Not solver error:
  - Solution spatially converges for inhomogeneous N_2-H_2-H_2O system.
  - Solution was validated for homogeneous H_2O system.
  - Solution is consistent with ODE solution for homogeneous N_2-H_2-H_2O system.

Likely Causes of Discrepancies

- Misinterpreting chemical reactions and rate constants from Ibe et al. [1].
- Neglecting additional physics considered by [1] (ex. gas bubbling).
- Typographic errors in chemical reactions and rate constants from [1].

Thank you for listening!