INL/CON-24-78918-Revision-0

FY24 All Hands Meeting: Understand and Predict Radiation-Induced Iodine Speciation, Chemistry, and Transport in High-Temperature Molten Salts

July 2024

Gregory Peter Holmbeck

Changing the World's Energy Future

Idaho National Laboratory

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17th July 2024

Brookhaven National Laboratory

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U.S. Department of Energy's Office of Nuclear Energy

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Molten salt reactors and fission product iodine

- Advanced nuclear reactor technologies are an integral part of the nation's future clean energy strategy.
- Molten halide salts are expected to play an important role as either coolant, fuel matrix, or pyrochemical separations media.
- **Iodine** is a **high-yield** fission product of concern for environmental release due to uptake in the human thyroid gland.
- Up to **70%** of the **iodine** generated in the 1975 *Molten Salt Reactor Experiment* (MSRE) could not be accounted for.

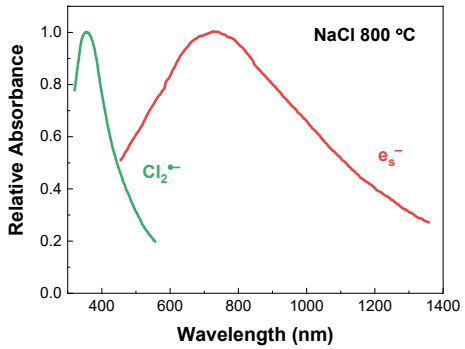
- Compere *et al.* Fission product behavior in the Molten Salt Reactor Experiment. ORNL-4865, **1975**.
- https://scitechdaily.com/the-future-of-nuclear-reactors-deciphering-electron-behavior-in-molten-salts/

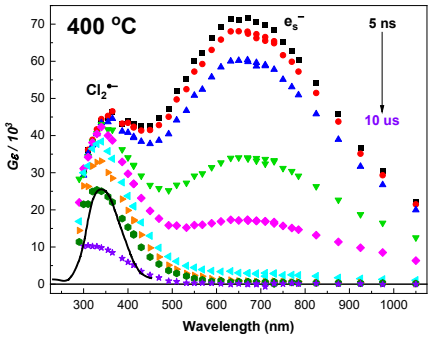
Molten salt radiation chemistry

Grimes, Chemical research and development for molten-salt breeder reactors, ORNL-TM-1853, 1967.

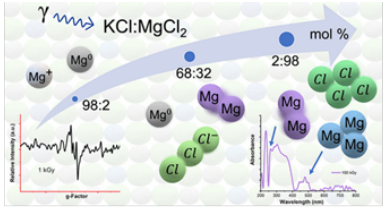
"...no major changes in the fuel or the Inconel which could be attributed to the irradiation conditions..."

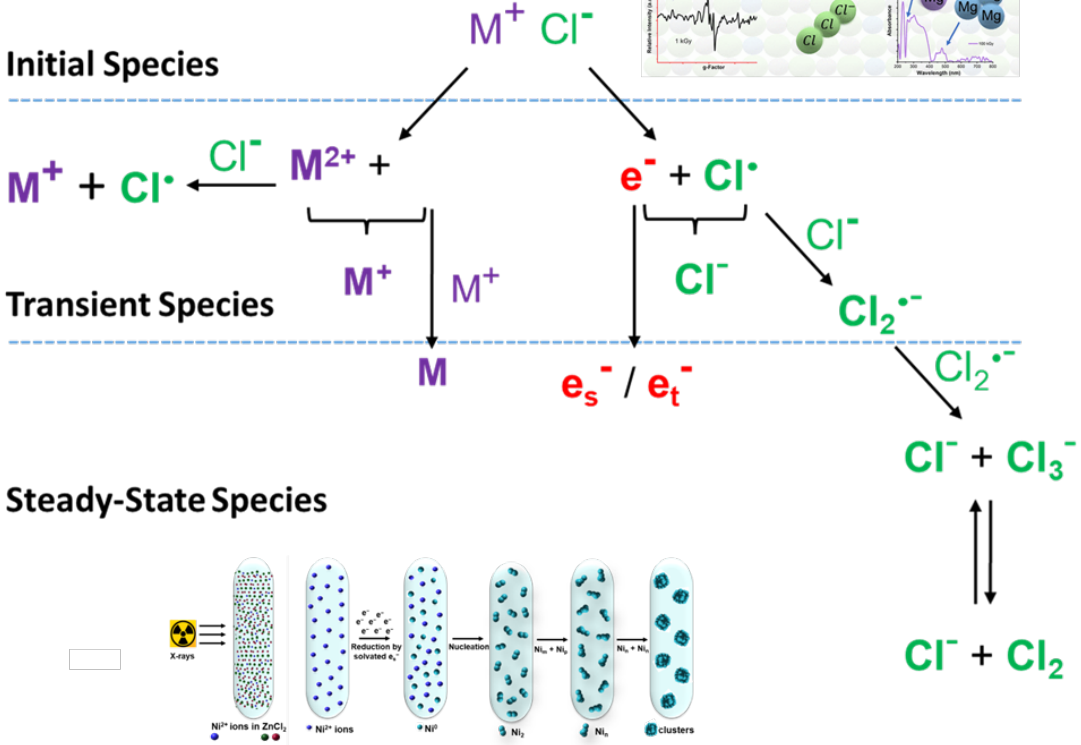
"...it was found that only when the irradiated fuel was allowed to freeze and cool below 100°C did radiolytic decomposition take place."





MSEE
molten salts in extreme environments





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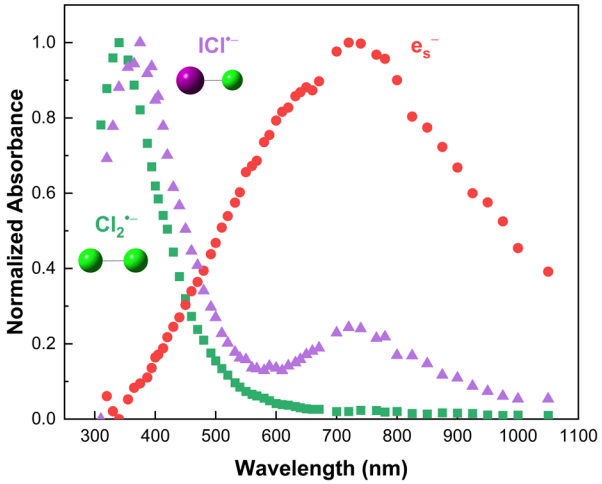
- Pikaev, Makarov, and Zhukova, *Radiat. Phys. Chem.* **1982**, *19*, 377.
- Iwamatsu, **Horne**, **Gakhar**, Halstenberg, Layne, Pimblott, and Wishart, *PCCP* **2022**, *24*, 25088.

Research goal

"To quantitatively understand and predict radiation-induced iodine speciation, chemistry, and transport in high-temperature molten salt environments"

Question: How does the absorption of ionizing radiation (**α**, **β**, and **γ**) change the chemical and physical properties of **iodine**-bearing molten salt systems?

Central hypothesis: The radiation-induced conversion of **iodide** will yield an extensive suite of **iodine** radiolysis products that will alter the bulk chemical and physical properties of the irradiated molten salt system—the *speciation*, *distribution*, and *chemical transport* of which will be dictated by the composition and the availability of multivalent metal cations and metal alloy interfaces.



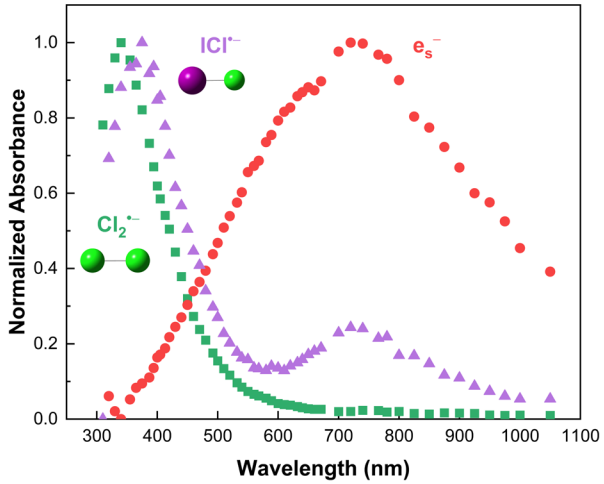
• **Conrad**, Iwamatsu, **Woods**, **Gakhar**, Layne, Cook, and **Horne**, *PCCP* **2023**, *25*, 16009.

Research objectives

Research objective #1: Determine how the inclusion of **iodine**/**iodide** influences the chemical and physical properties of complex molten salt mixtures in the absence of ionizing radiation fields.

Research objective #2: Understand the speciation and fundamental chemical behavior of transient and “steady-state” **iodine**/**iodide** species formed by the irradiation of molten and solid salt mixtures.

Research objective #3: Evaluate the influence of interfacial processes on determining the final disposition of **iodine** in high temperature molten salts, notably the structure and chemical speciation of **iodine** at metal-salt interfaces.



• **Conrad**, Iwamatsu, **Woods**, **Gakhar**, Layne, Cook, and **Horne**, *PCCP* **2023**, *25*, 16009.

Program aims and progress (FY23 → FY24)

- ☑ Identify and characterize the suite of radiation-induced **iodine** species formed in high-temperature molten salt mixtures
- ☑ Determine their impact on the bulk chemical and physical properties of a molten salt mixture
- ☑ Elucidate their reaction kinetics, mechanisms, and chemical transport as a function of temperature and base salt composition
- ☑ Evaluate their interplay with multivalent metal ions and metal alloy interfaces
- ☐ Develop multiscale computer models for the interrogation and prediction of reaction mechanisms, speciation, and chemical transport in irradiated, high-temperature **iodine**-bearing molten salts.

• **Conrad**, Iwamatsu, **Woods**, **Gakhar**, Layne, Cook, and **Horne**, *PCCP* **2023**, *25*, 16009.

FY23 research team

FY24 research team additions

Stephanie Castro Baldivieso

INL Glenn T. Seaborg Distinguished Postdoctoral Research Associate

Electrochemistry and electrode materials design

Insung Han

BNL Postdoctoral Research Associate

Metal solidification and X-ray image analysis

Kyle Halloway

INL GEM Fellow

Advanced materials characterization

Qiufeng Yang

INL Postdoctoral Research Associate

Electrochemical corrosion in molten salts

Priyanshi Agrawal

INL Postdoctoral Research Associate

Advanced materials characterization

Linu Malakkal

INL Early Career Researcher

Modeling and simulation of material behavior in nuclear fuels and structural materials

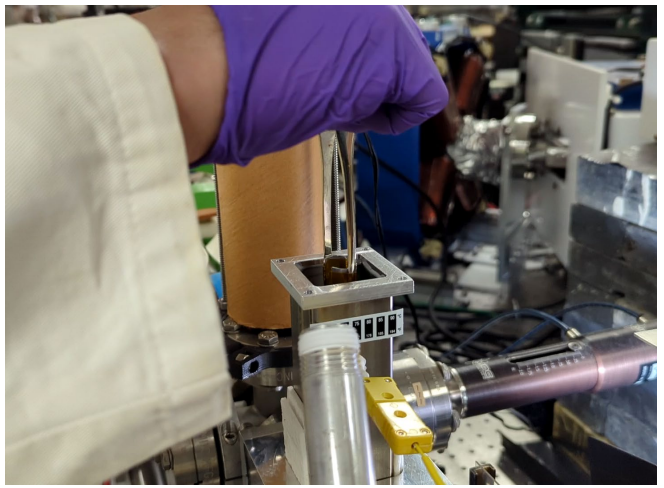
Corey Pilgrim

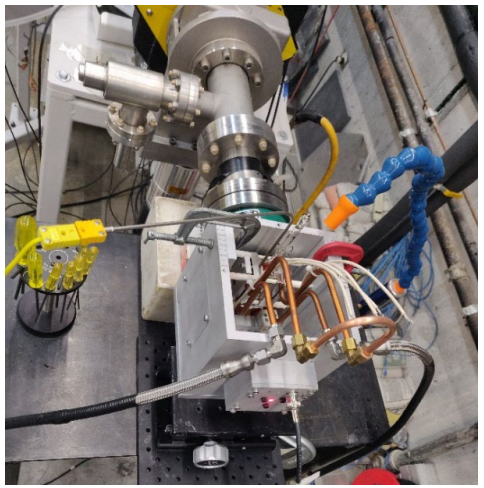
INL Early Career Researcher

Nuclear magnetic resonance spectroscopy

FY24 productivity

- Awards (1)
- New Capabilities (2)
- Publications in Preparation (5)
- Publications in Review (1)
- Scientific User Facility Awards (8)
- Synergistic Activities (1)
- Technical Presentations (12)
- Workforce Development (3)





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