A Simulation Surrogacy Method For The Study Of Molten Salt Reactor Lifecycle Chemistry

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Background

Understanding the chemical behavior of fuel salt throughout a Molten Salt Reactor's (MSR) lifecycle is key to determining:

- Optimal Fuel Cycling
- Radiological Risk
- Fouling of Heat Exchangers

With limited thermochemical data for impurities in irradiated fuel salt, **this work proposes a framework to model MSR chemistry, using simulation surrogates for elements lacking data**.

Methodology

Suitable surrogates will have similar chemical behavior. The first surrogate mapping makes use of similarities between half reactions and valence states.

Surrogate: An element for which data is readily available in MSTDB-tc v3.1

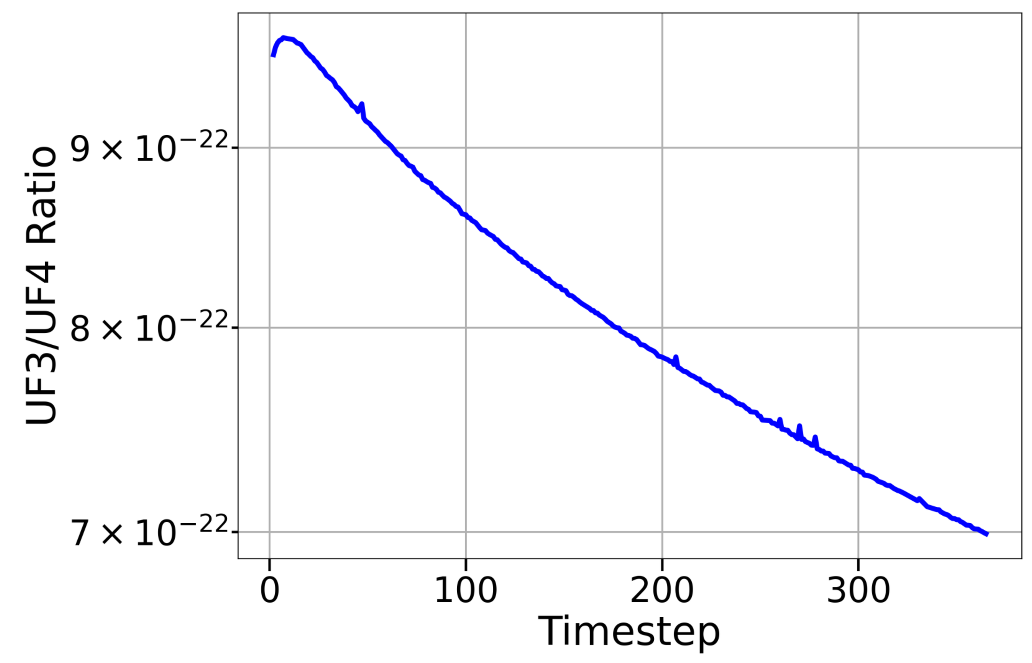
Candidate: An element for which no data is available in MSTDB-tc v3.1

Some have no suitable surrogate.

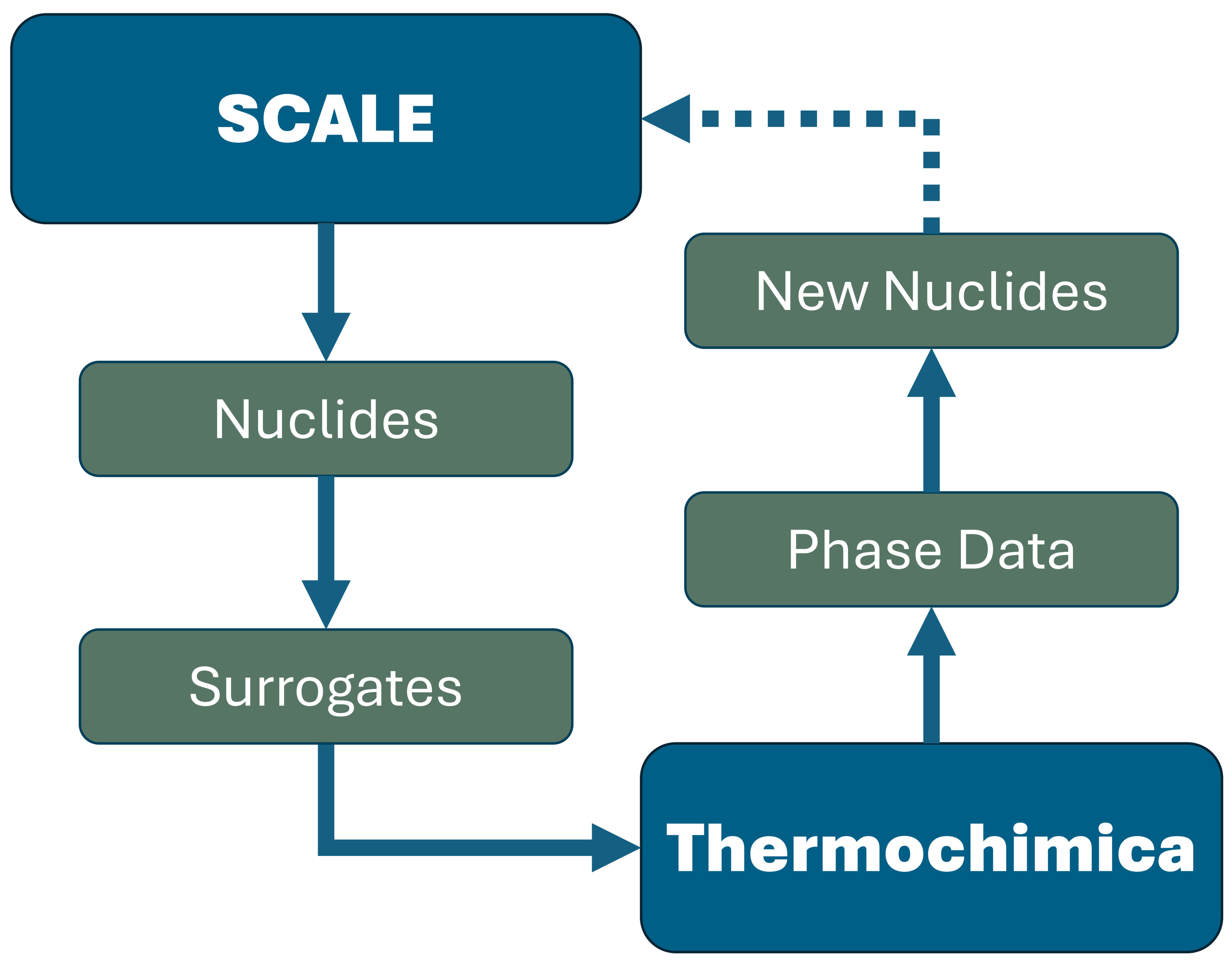
Framework

- **SCALE** – Runs Depletion Calculations
- **Thermochimica** – Gibs Energy Minimizer (using MSTDB)
- **Molten Salt Thermochemical Database** (MSTDB)

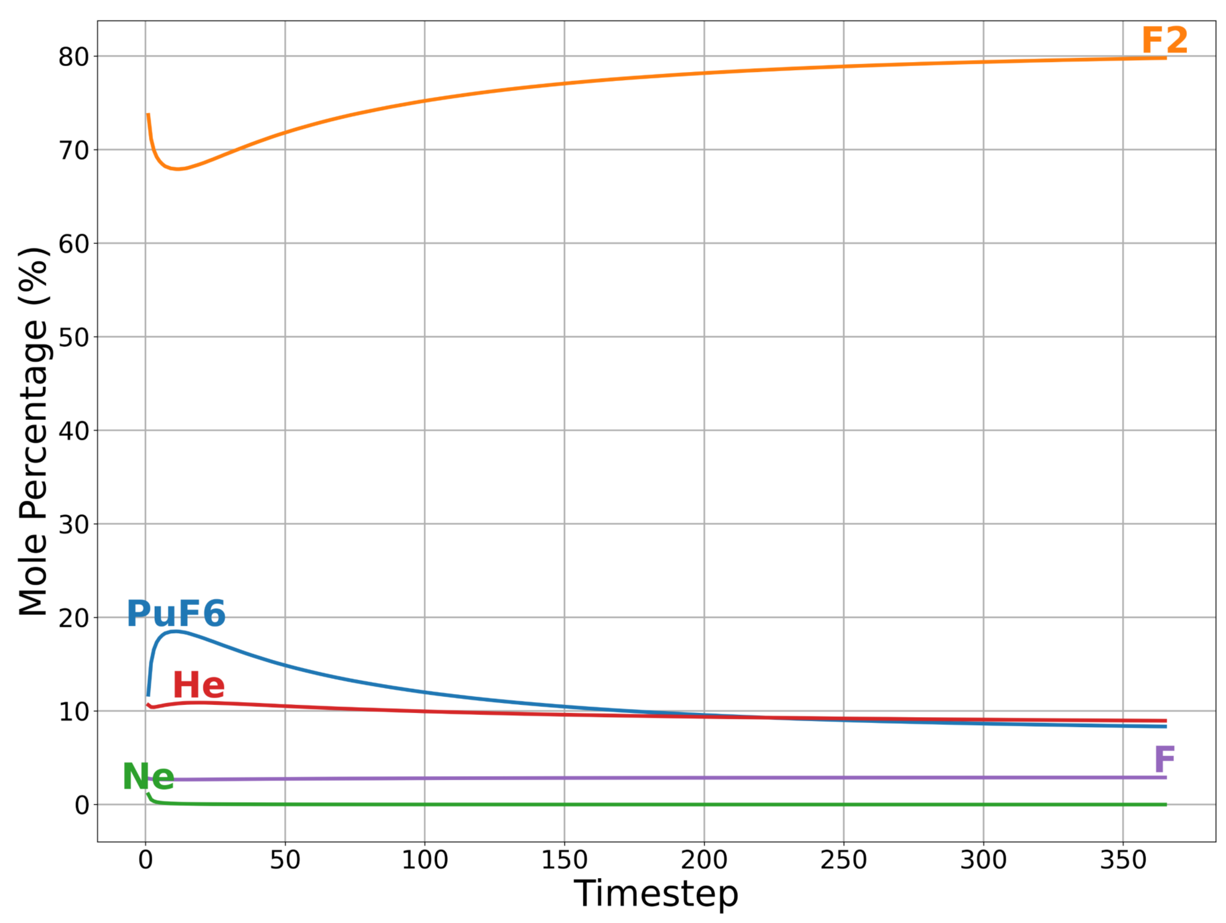
Findings



- Chemistry Control needed to keep salt healthy (~ 0.0001 – 0.01 UF_3/UF_4)



SCALE_2_Thermochimica Framework



- Uncontrolled salt produces volatile species such as F_2 and PuF_6
- ThEIRENE Fuel Cycle: 0.002 moles of additional gas per mole salt

Conclusions

- MSTDB offers many important capabilities, but has no data for key species: O, H, Te
- Introducing I with other impurities creates numerical instabilities and non-physical results
- Chemical control is needed to mitigate fluorine volatility.
- It is vital that adaptable frameworks be built so that new data can be easily incorporated

Future Work

- Improved Surrogate Mapping
- Iodine Sensitivity Studies
- Physics Based Separation Schemes
- Investigation of Redox Controls
- Improve Framework Efficiency
- Complete Timestep Integration

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