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U.S. DEPARTMENT OF ENERGY | Office of NUCLEAR ENERGY

Molten Salt Reactor PROGRAM

MSR Species Tracking Modeling & Simulation

Idaho National Laboratory

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Annual MSR Campaign Review Meeting 2-4 May 2023

PART-I: INL Scope

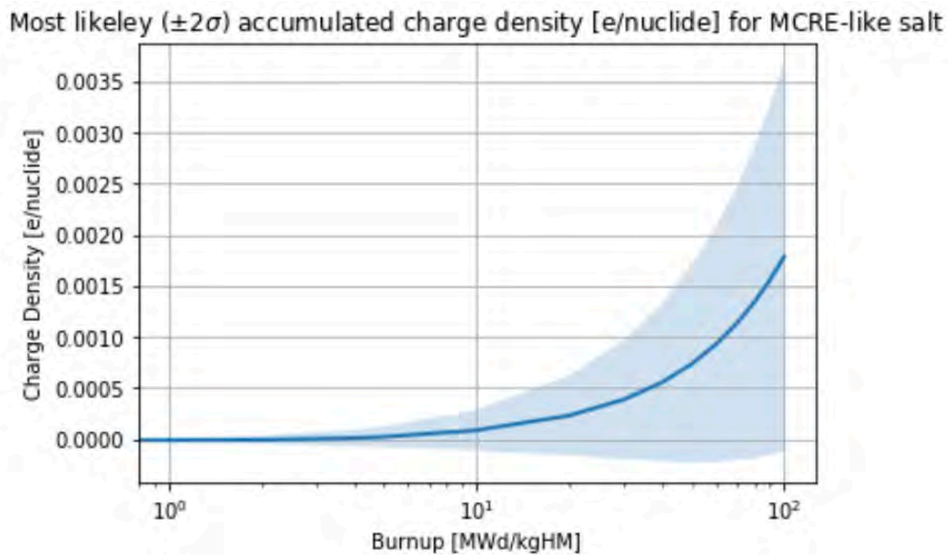
Multiphysics Depletion and Species Tracking using NEAMS Tools

Overview:

1. Background
2. Updating FY22 0D Depletion + Thermochemistry Model
3. 2D/3D Depletion + Advection
4. Advection + Thermochemistry
5. Progress on Depletion + Advection + Thermochemistry

Why Does it Matter?

- **Importance of Species Tracking**
  - **Containment**: Where do the radionuclides go? What is the reactor source term?
  - **Heat removal**: Where do isotopes plate out? How do we cool the reactor?
  - Reactivity: Where do the neutron precursors go? What is the reactor beta-eff?
  - Corrosion: How do fission products interact with the wall? How long will a barrier last?
  - Safeguards: Where do the fissile isotopes go? How do we monitor where they are?
- **Methodology**
  - Collect data and populate MSTDB → Ongoing
  - Develop models that leverage data to estimate, based on reactor design parameters, the behavior of species within an MSR → This work
- **Benefits:**
  - Inform designers on source term, decay heat, controllability, corrosion, and safeguards
  - Inform experimentalists of equipment sensitivity & research priorities

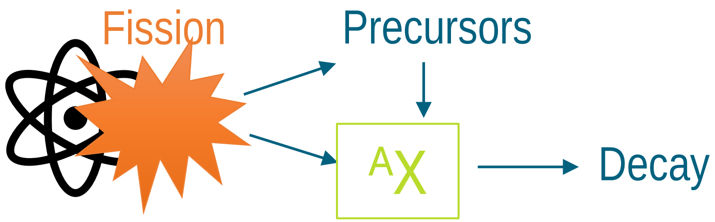


Leveraging NEAMS Tools

Nuclear Energy Advanced Modeling and Simulation

Physics to Capture:

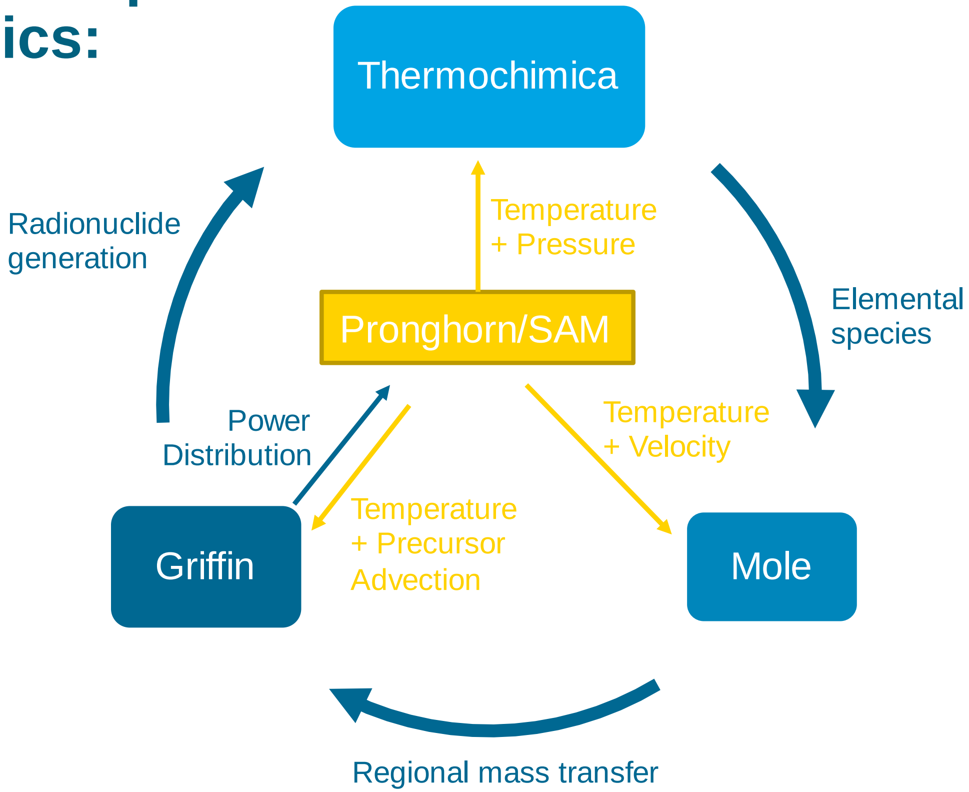
- Neutronics:



- Thermal Hydraulic:

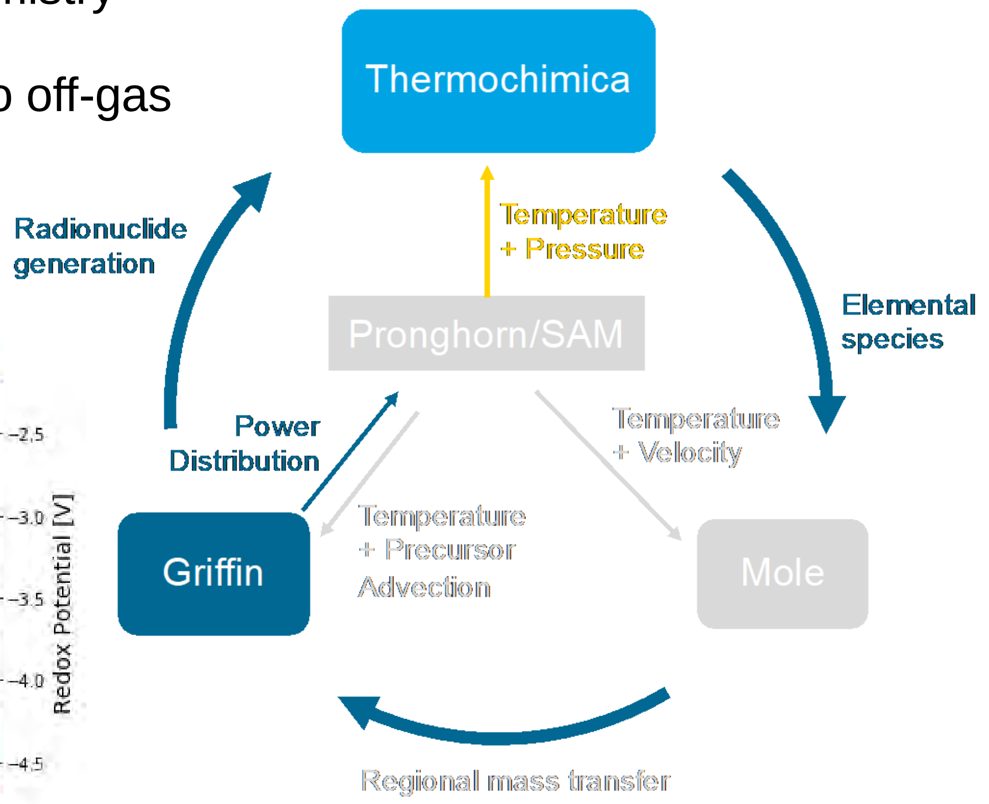
- Thermochemical effects:
  - Speciation (e.g., formation of gaseous I species)
  - Volatilization (at liquid-gas interface)
  - Bubbling (transfer of Cs to He gas bubbles)
  - Precipitation (solid U compound phase)

Tools that Capture the Physics:

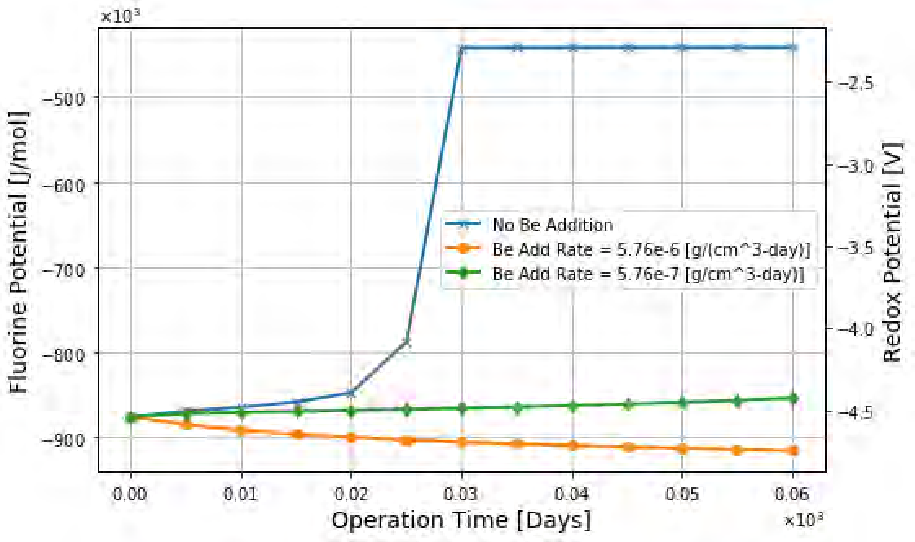


Step 1: Depletion + Thermochemistry

- 0D approximation capturing depletion (Griffin) and thermochemistry (Thermochimica) developed by NEAMS in FY22
- 2-Region CRAM solver to remove volatile species from core to off-gas
- Specify removal rate (provided by other code)
- Updated FY22 analysis using MSTDB-TC v2.0
- Redox control by addition of reducing metals into system



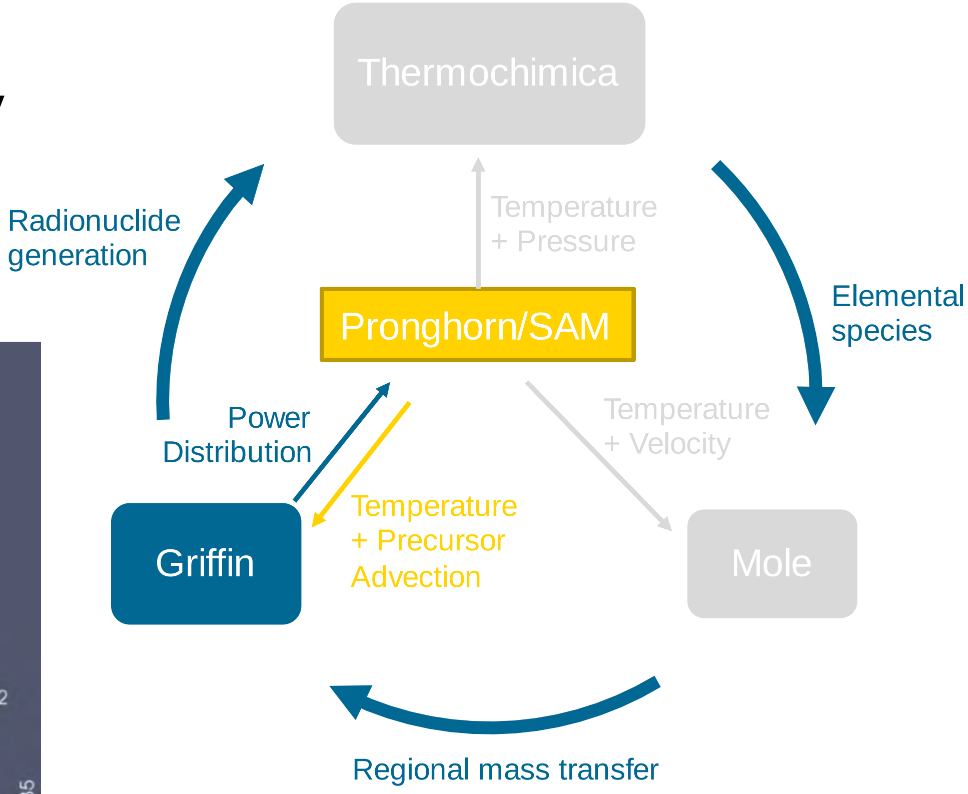
Removal (Yes/No)	^{131}I – Core [atoms/b-cm]	^{131}I – OG [atoms/b-cm]
No	9.462e-09	0.0
Yes	9.432e-09	5.883e-17
% Difference	0.32%	



Publications:
- **ICAPP 2023**: “Leveraging Coupled Thermochemical Depletion Capabilities to Evaluate Off Gas and Source Term Characterization in Molten Salt Reactor Systems”
- **Frontiers Journal (submitted)**: “Depletion Driven Thermochemistry of Molten Salt Reactors: Method, Analysis, and Impact”

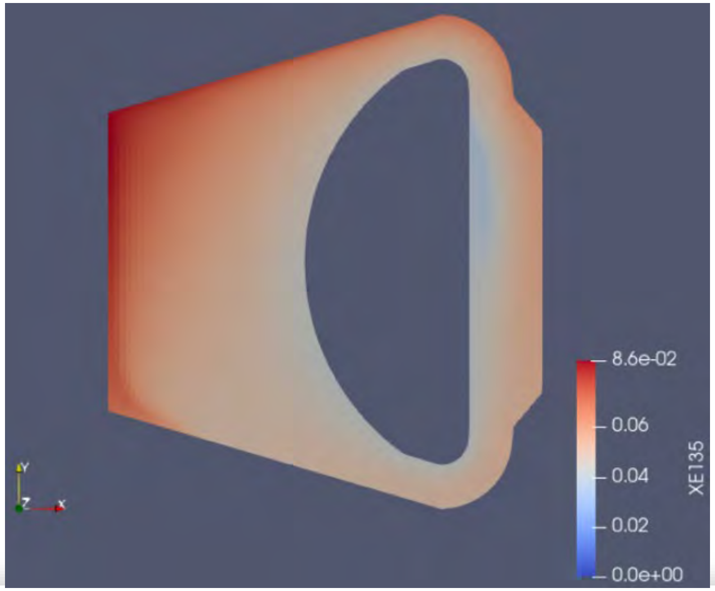
Step 2: Depletion + Advection

- New depletion capability in Griffin developed by NEAMS to account for isotopes born in core but decaying outside
- To make problem tractable: only applies to isotopes that decay not too quickly (stay in core) and not too slowly (well mixed)
- Ignoring this advection effect can lead to substantial errors at specific removal values



Removal rates	^{135}Xe – OG [atoms/(b-cm)]	Percent Diff. from 0D Calculation
$r = 0.10$	1.304e-07	0.77%
$r = 0.01$	1.251e-07	4.40%
$r = 0.001$	5.595e-08	20.59%

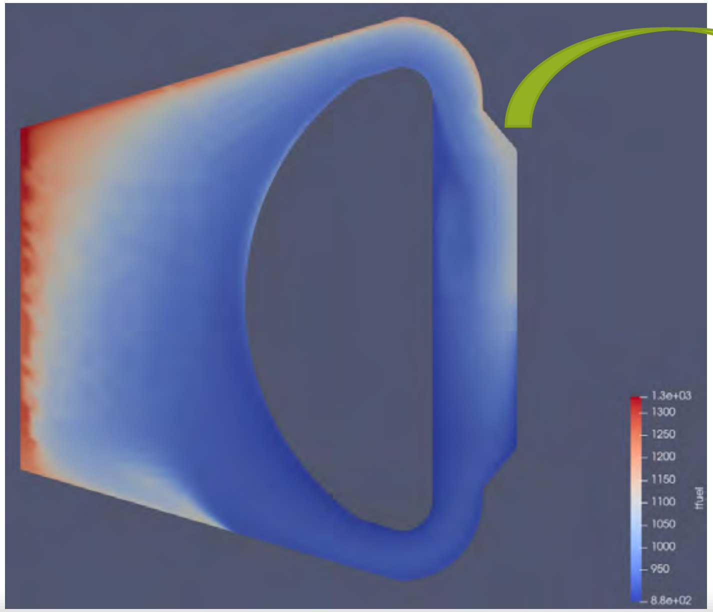
Publications:
- **ICAPP 2023**: "Spatially Resolved Depletion Studies of Circulating Fuel Molten Salt Reactor Systems"



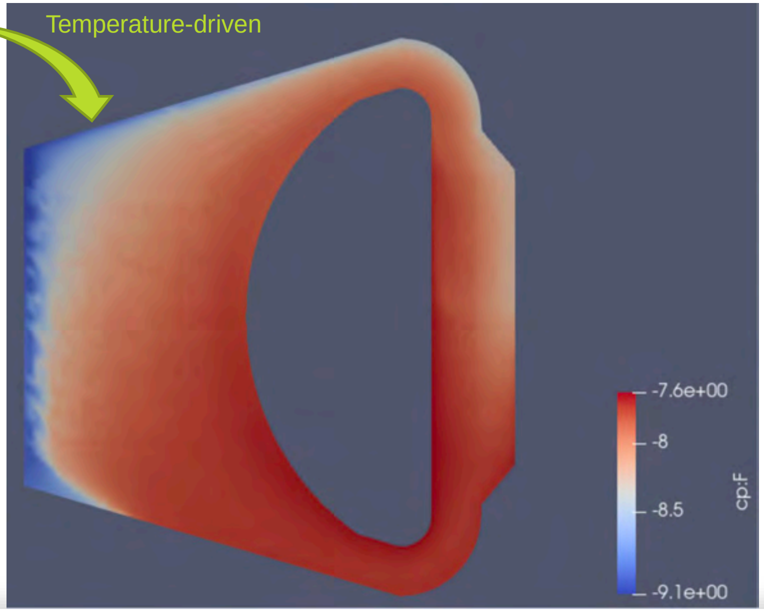
^{135}Xe concentration distribution with $r = 0.1\frac{1}{s}$.

Step 3: TH + Thermochemistry

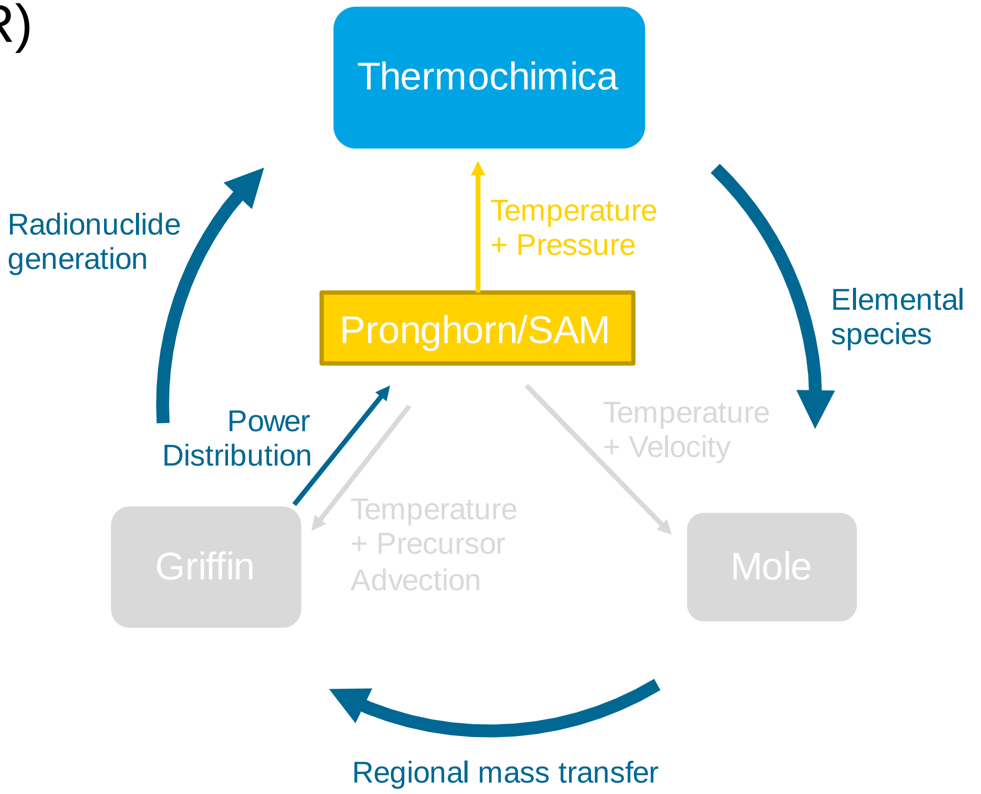
- Accounting for variability in thermochemistry and speciation throughout reactor flow and temperature field (ART-MSR)
- Evaluate chemical potential of species within spatial distribution (temperature-driven)
- Ongoing work: importing species phases (NEAMS)



Temperature of Molten Salt

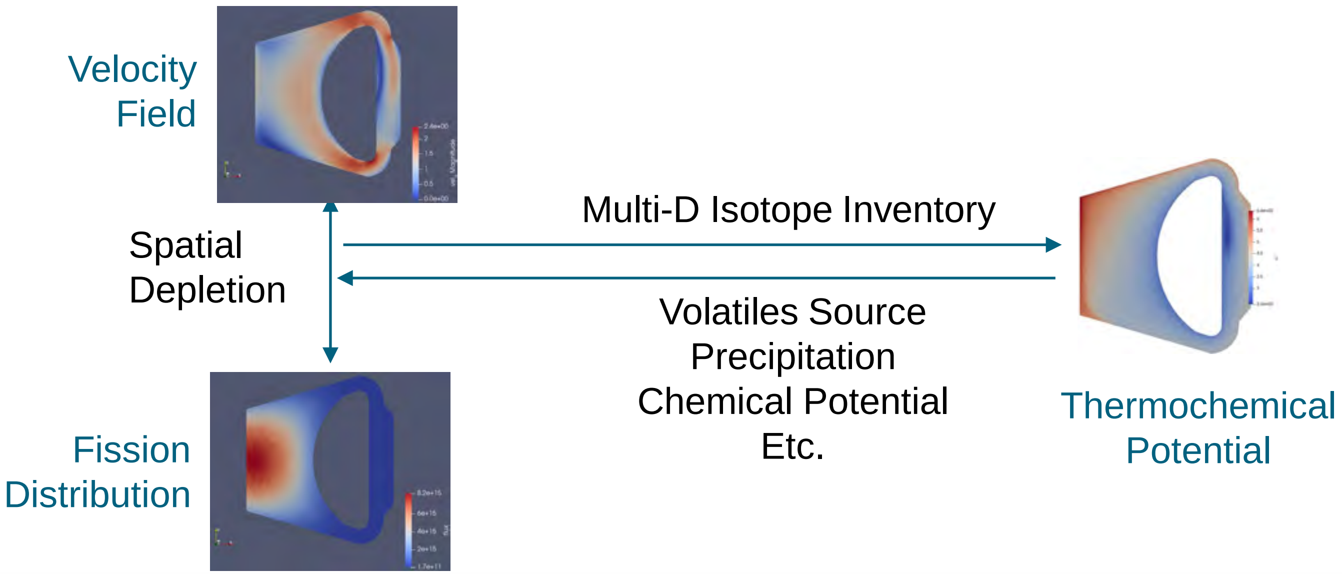


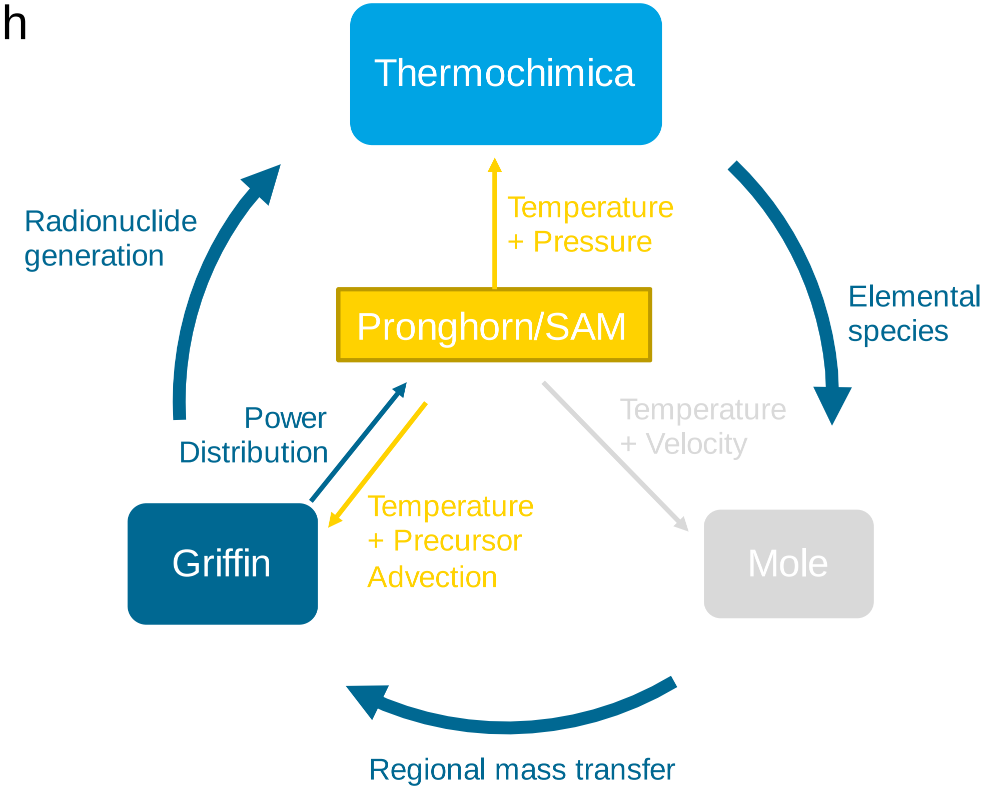
Chemical Potential of Fluorine



Step 4 (Ongoing) : Depletion + TH + Thermochemistry

- Bringing it all together: deplete isotopes (Griffin), move through salt (Pronghorn), evaluate speciation (Thermochimica)
- First step: evaluate off-gasing of species
- Second step: evaluate precipitation of species
- Missing physics: regional mass transfer (Mole)





Next Steps

This FY

- Complete step 4 model
- Leverage to predict 3D resolved off-gasing and precipitation rates of nuclides
- Compare MELCOR against NEAMS → **SNL collab**
- Feed MELCOR correlations → **SNL collab**

Next FY

- Include Mole into framework → **ORNL collab**
- Improve off-gas and precipitation models with Two-Phase bubbling model
- Incorporate corrosion dynamics
- Establish NEAMS-MELCOR workflow for Accident Transient Analysis

SNL-INL Status:

	Thermal F MSR	Fast Cl MSR
INL	• MSRE Griffin model complete • Pronghorn model under dev • Apply framework once Griffin-Pronghorn model established	• Reference model already built • Framework partially established • First use case for comprehensive species tracking capability
SNL	• MELCOR model established • Incorporate ORIGEN-based depletion capabilities • Obtain vapor pressure correlations from NEAMS	• Develop Cl based equations of state • Build reference Cl MSR model • Obtain vapor pressure correlations from NEAMS

Thank you

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