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Molten Salt Reactor PROGRAM

Species Tracking in Molten Salt Reactors

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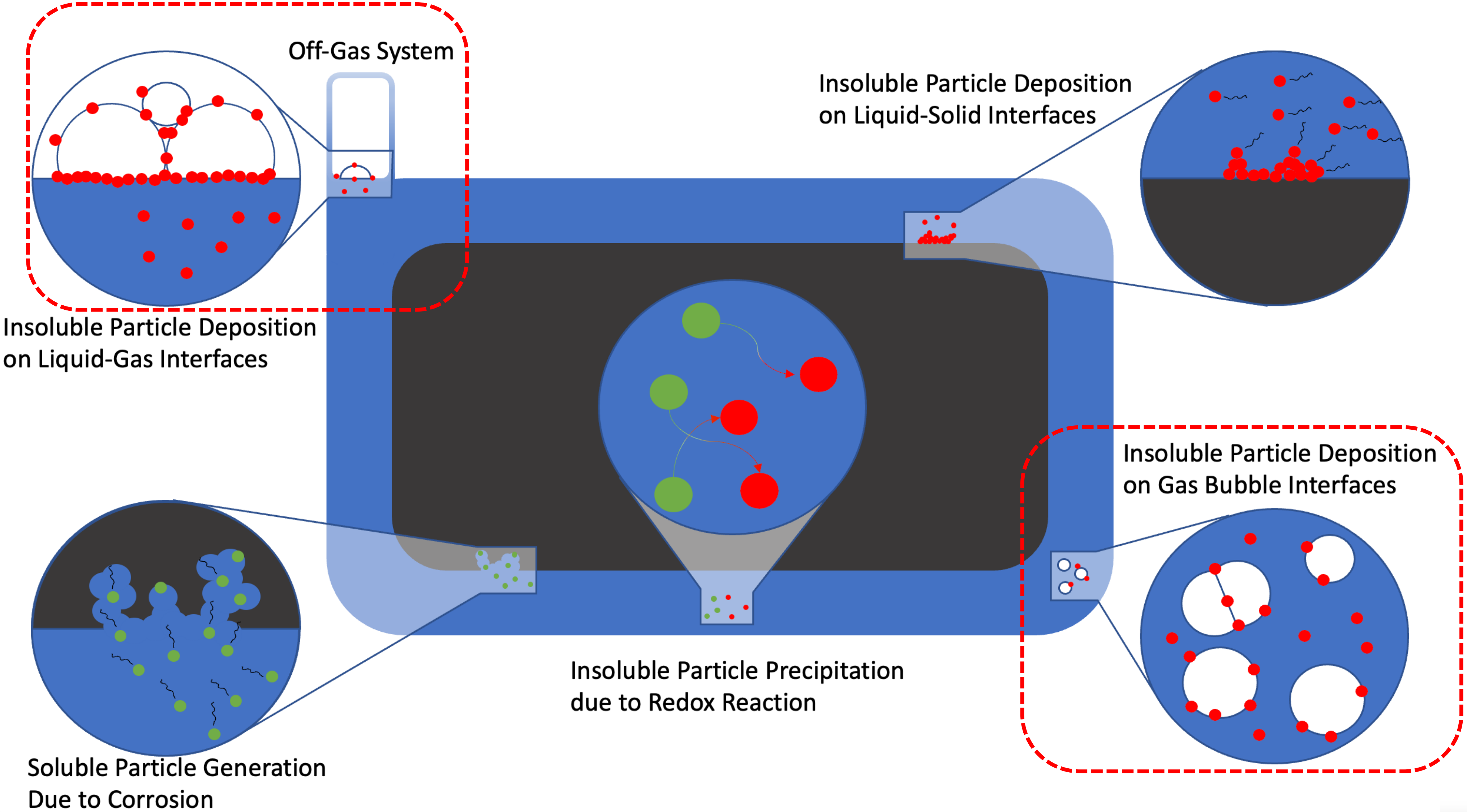
Content

1. **Motivation for species tracking in MSRs**
2. **Development of a computational framework for species tracking**
3. **FY24 scope: coupled transport of soluble + gaseous species**
4. **Application example to Molten Salt Reactor Experiment**

Species Tacking Behavior in MSRs



Off-Gas System

Insoluble Particle Deposition on Liquid-Solid Interfaces

Insoluble Particle Deposition on Liquid-Gas Interfaces

Insoluble Particle Deposition on Gas Bubble Interfaces

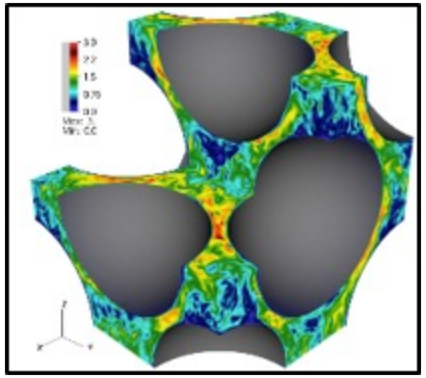
Insoluble Particle Precipitation due to Redox Reaction

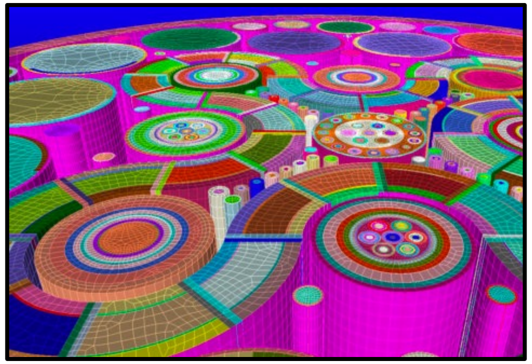
Soluble Particle Generation Due to Corrosion

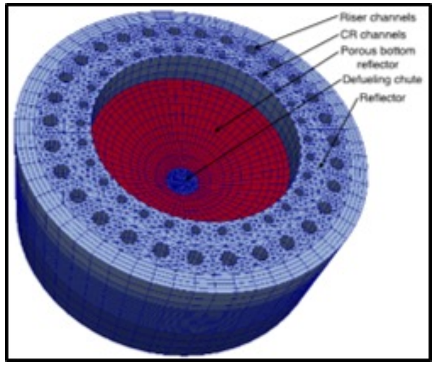
Why do we need to track species?

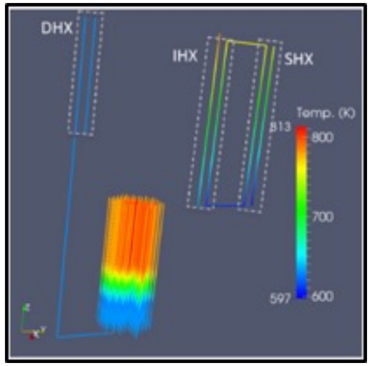
- Importance of Species Tracking
  - **Containment**: Where do the radionuclides go? What is the reactor source term?
  - **Heat removal**: Where do isotopes plate out? How do we cool the reactor?
  - **Reactivity**: Where do the neutron precursors go? What is the reactor β_{eff}?
  - **Corrosion**: 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?

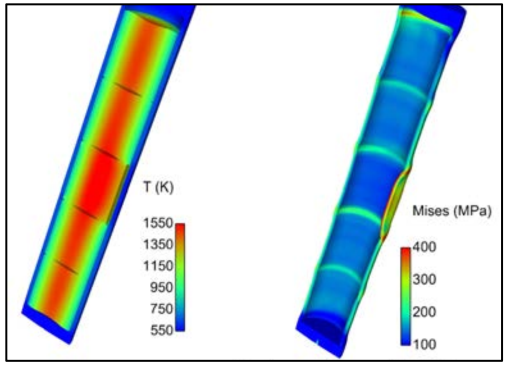
Main NEAMS tools used for modeling and simulation of MSRs











Nek-5000 nekRS + **Griffin** + **Pronghorn** + SAM + BISON/ Thermochimica

Fuel Performance/ Thermochemistry

High Fidelity- Physics Resolved

Component Scale

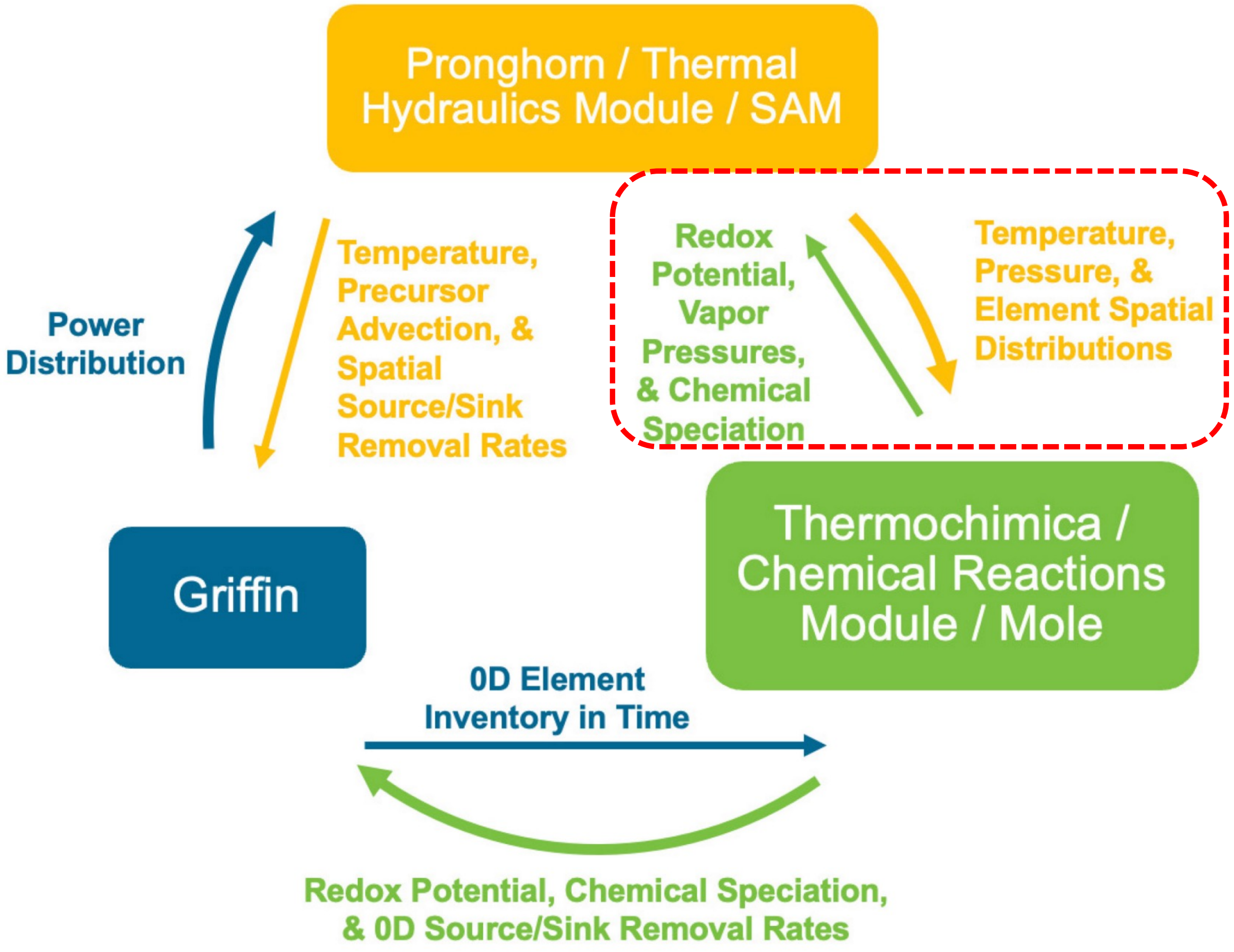
Plant Scale

Operation Analyses

Coupling framework for species tracking

- The coupling framework for species tracking in MSRs involves:

1. **Griffin**: neutronics + depletion
2. **Pronghorn**: thermal-hydraulics + species transport
3. **Thermochimica**: chemical equilibrium calculations



FY23 work: framework coupling for evaluating soluble fission product retention

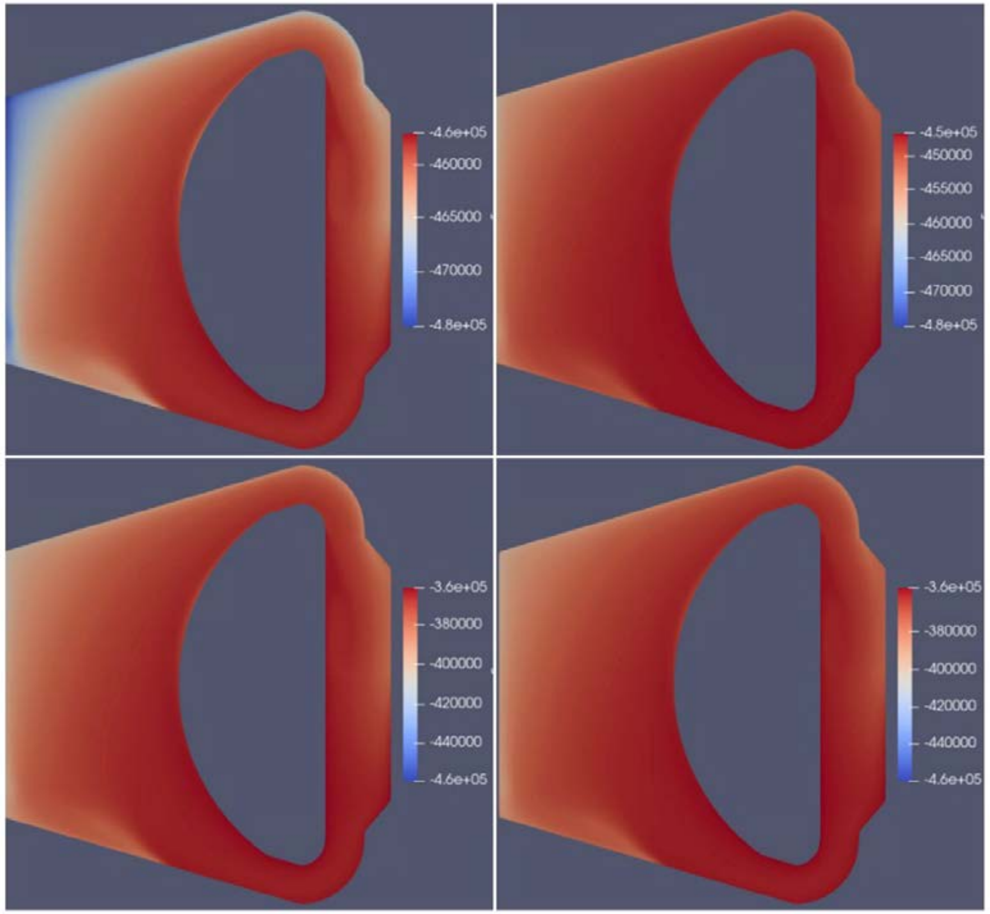


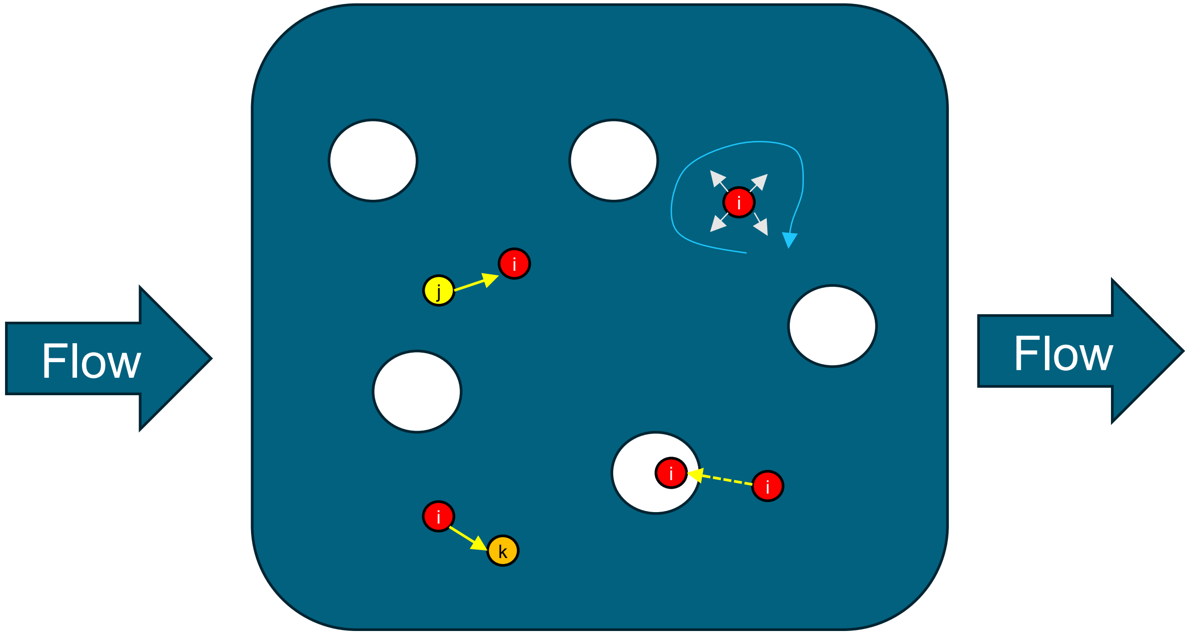
Figure 6-2. Fluoride (F-) potential (J/mol) at (clockwise, from upper left) 0.024, 0.048, 0.096, and 0.239 MWd/Kg-U, showcasing the oxidizing effect of depletion on MSFR fuel salt.

Removal rates	^{137}Xe – Core [atoms/(b-cm)]	^{137}Xe – OG [atoms/(b-cm)]	Percentage in OG
$r = 0.10$	2.202e-11	7.280e-10	97.06%
$r = 0.01$	1.742e-10	5.758e-10	76.77%
$r = 0.001$	5.637e-10	1.863e-10	24.84%
	^{137}Cs – Core [atoms/(b-cm)]	^{137}Cs – OG [atoms/(b-cm)]	Percentage in OG
$r = 0.10$	2.391e-07	2.279e-06	90.50%
$r = 0.01$	7.101e-07	1.802e-06	71.73%
$r = 0.001$	1.904e-06	5.830e-07	23.44%

- Speciation and mass balances affects by the evolution of 3D chemical potential
- It is key to consider multi-D fields (temperature, pressure, composition, etc.) in MSRs
- **We need to better account for the transport of gaseous species**

FY24: Coupled transport of soluble + gaseous species

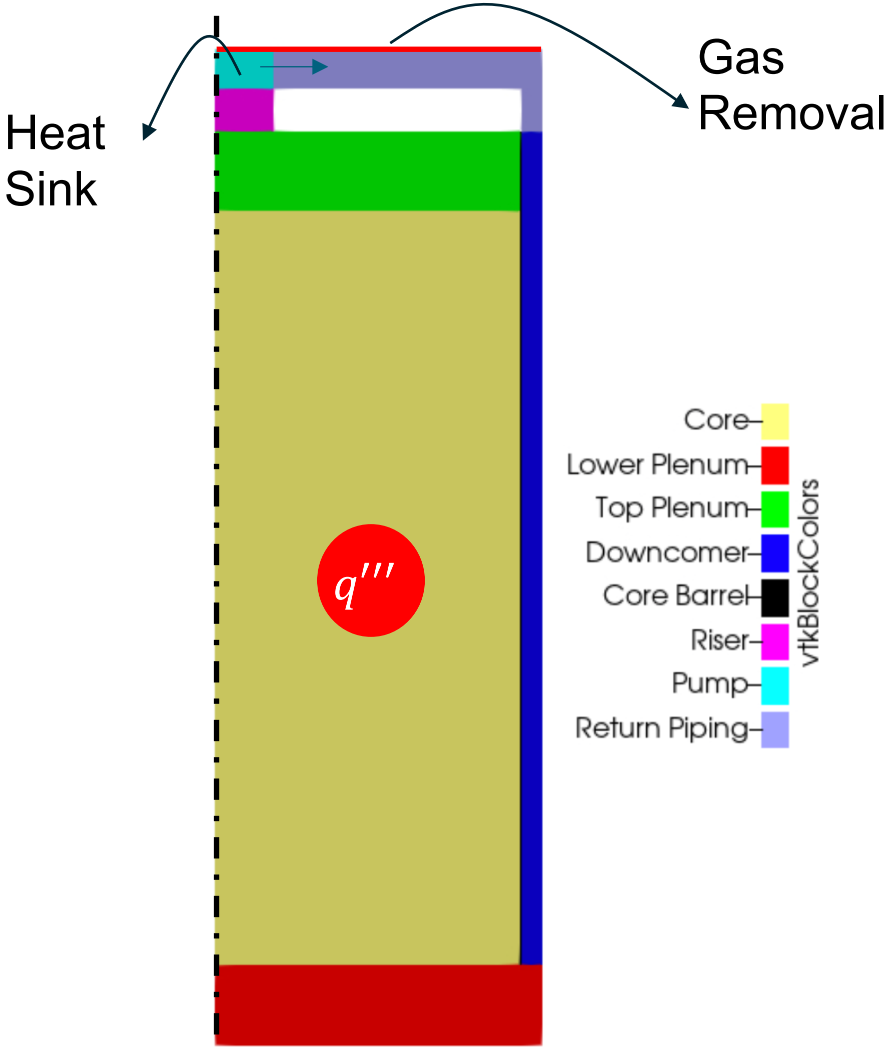
- 🟦 Fuel Salt
- ○ Bubbles
- i Isotopes of kind i
- j Isotopes of kind j
- k Isotopes of kind k



$$\underbrace{\frac{\partial c_i^x}{\partial t}}_{\substack{\text{Time}\\ \text{derivative}}} + \underbrace{\nabla\cdot\left(\frac{\boldsymbol{u}}{\gamma}c_i^x\right)}_{\substack{\text{Convection in}\\ \text{Porous Media}}} - \underbrace{\nabla\cdot\left[\left(D_{C_i}+\frac{\nu_t}{Sc_t}\right)\nabla c_i^x\right]}_{\substack{\text{Molecular and}\\ \text{Turbulent Diffusion}}} = \underbrace{y_i f}_{\substack{\text{Fission Yield}\\ \text{Source}}} - \underbrace{\lambda_i^{eff} c_i^x}_{\substack{\text{Effective}\\ \text{Decay Sink}}} + \underbrace{\lambda_{j\to i}^{eff} c_j^x}_{\substack{\text{Effective}\\ \text{Transmutation}\\ \text{Rate}}} - \underbrace{h^{xy}\left(c_i^x - c_i^y\right)}_{\substack{\text{Exchange of phases}\\ \text{between states y and x}}}$$

Application to MSRE

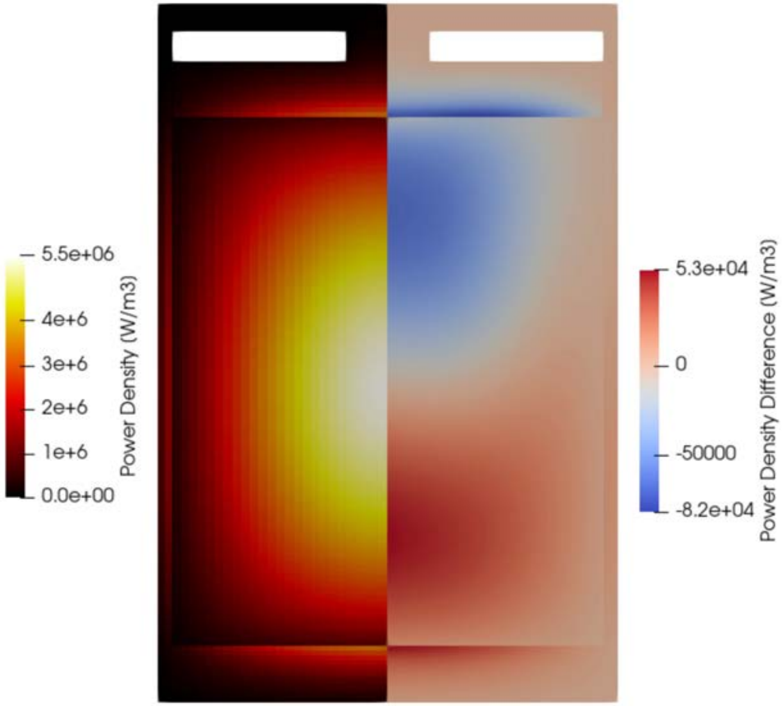
- Model application to 2D axisymmetric model of Molten Salt Reactor Experiment (MSRE)
- Pump above riser circulates the fuel salt
- Fission power is produced at the center of the core with a total power of 10MW
- A heat sink simulating the heat exchanger is placed at the pump location
- All gases are extracted with an assumed 100% efficiency at the top boundary



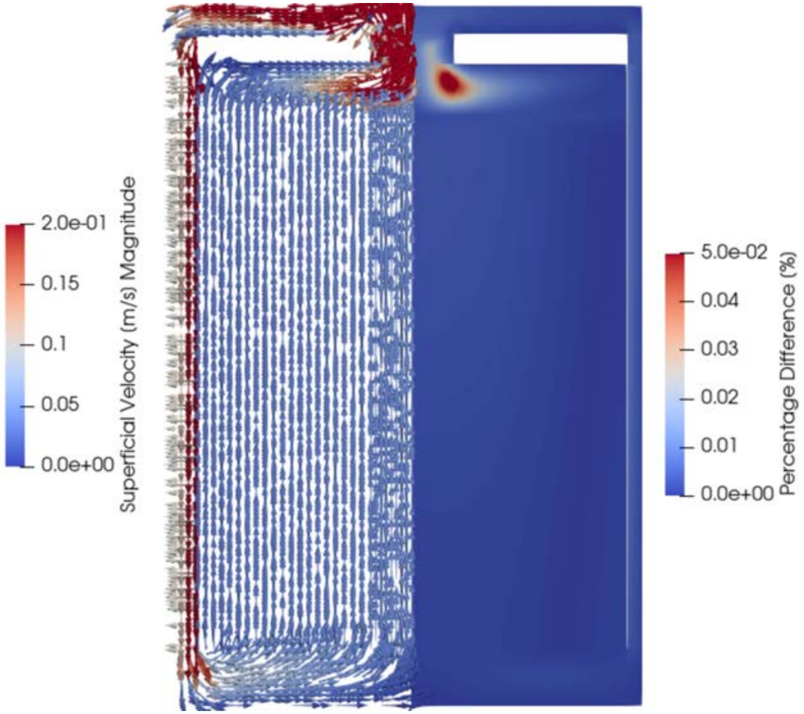
Example: Molten Salt Reactor Experiment Axisymmetric Model

MSRE – Steady-State Operation

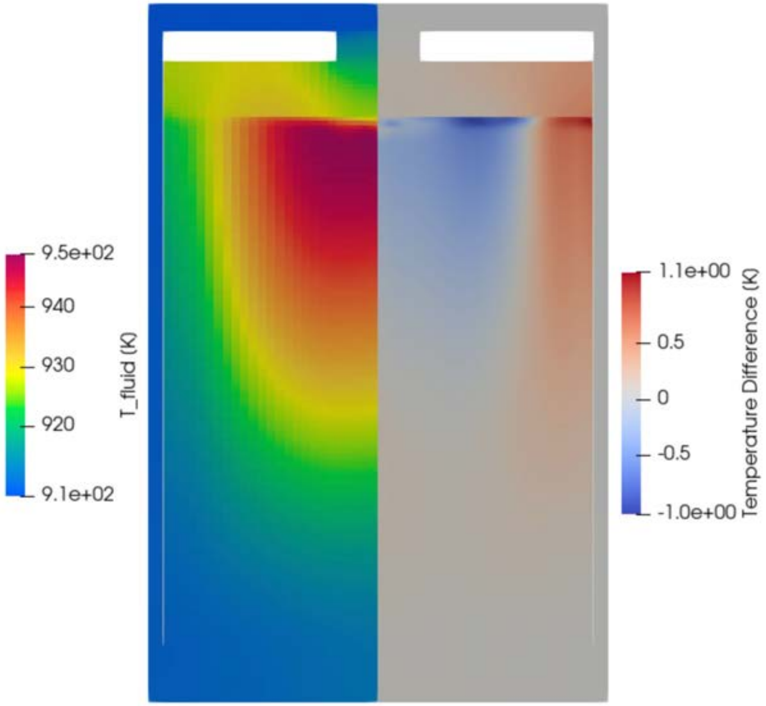
Impact of void transport modeling



Power Density Shift



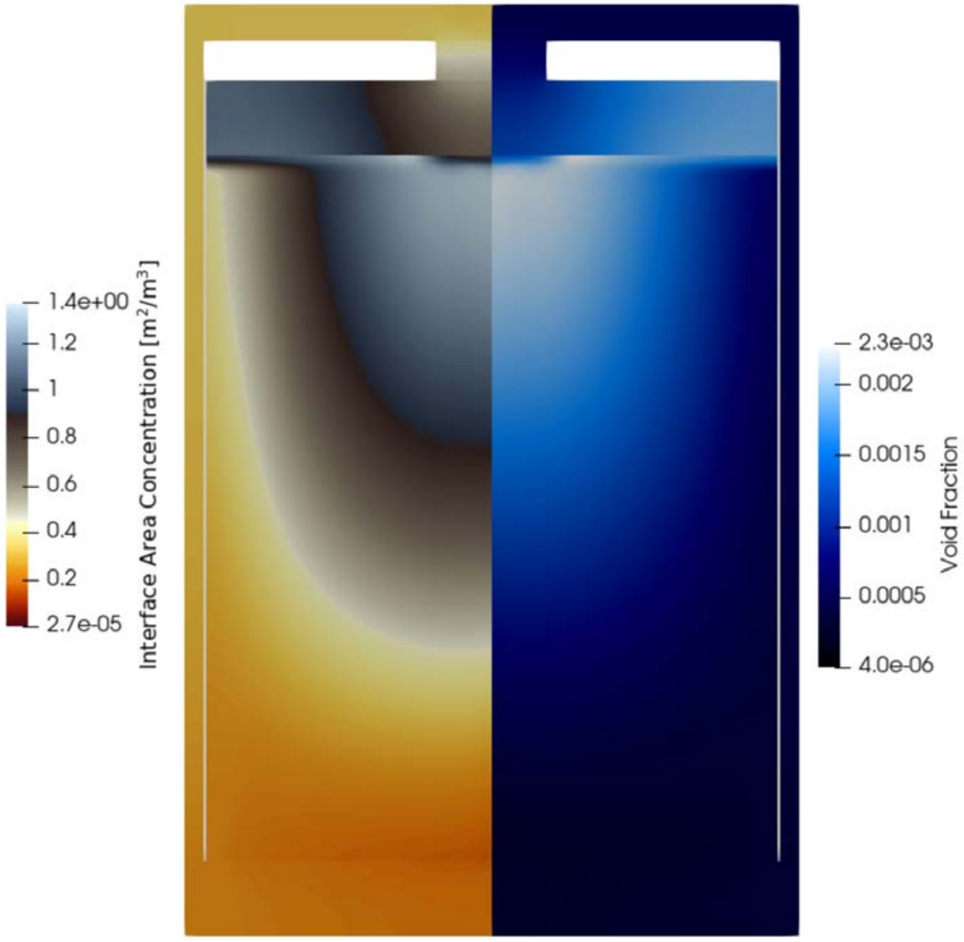
Velocity Shifts



Temperature Changes

Void Distribution

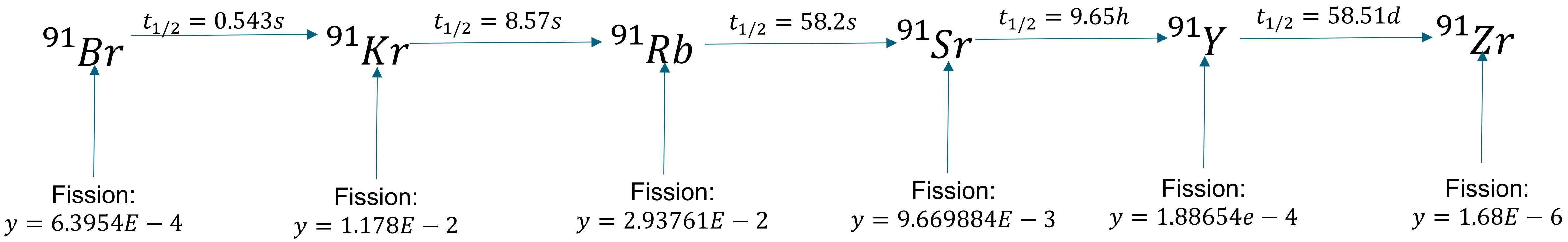
- Void increases as the fuel circulate through the reactor core
- As flow mixes in the upper plenum two different behaviors are observed:
  - Flow jets to the riser, where void is removed at the pump
  - Flows is more occluded towards the external radius of the upper plenum, resulting on a higher void concentration
- Interface area concentration and hence, liquid-gas exchange processes are larger at the top of the core and the partially occluded flow in the outer radius of the upper plenum



Example: Steady-State void distribution

Demonstration problem

- Tracking the depletion chain of ^{91}Br



$^{91}Br \xrightarrow{t_{1/2} = 0.543s} {}^{91}Kr \xrightarrow{t_{1/2} = 8.57s} {}^{91}Rb \xrightarrow{t_{1/2} = 58.2s} {}^{91}Sr \xrightarrow{t_{1/2} = 9.65h} {}^{91}Y \xrightarrow{t_{1/2} = 58.51d} {}^{91}Zr$

Fission: $y = 6.3954E - 4$

Fission: $y = 1.178E - 2$

Fission: $y = 2.93761E - 2$

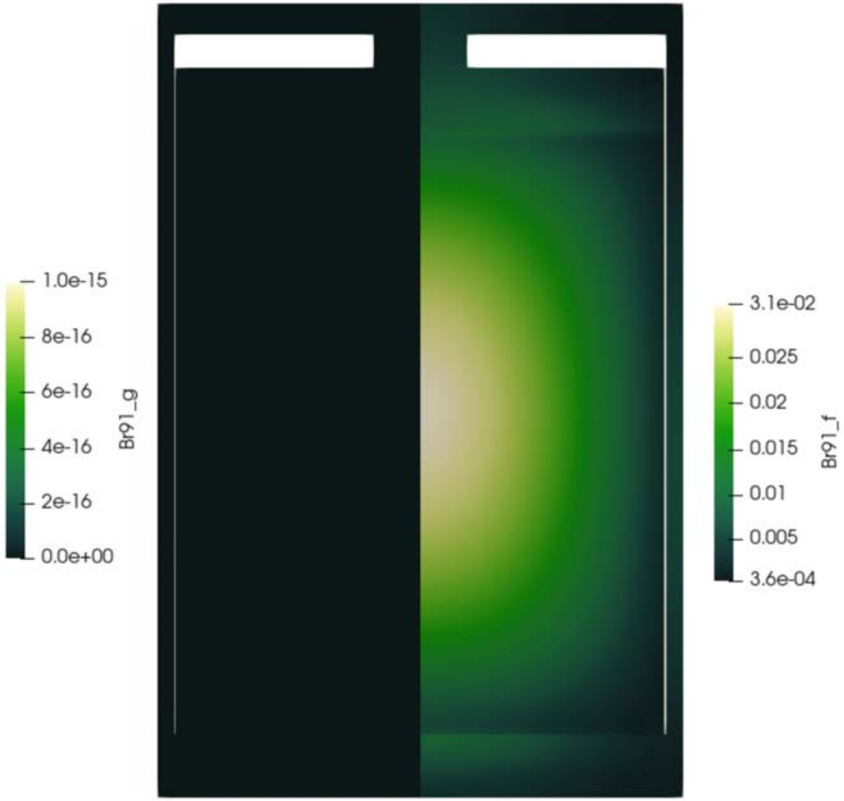
Fission: $y = 9.669884E - 3$

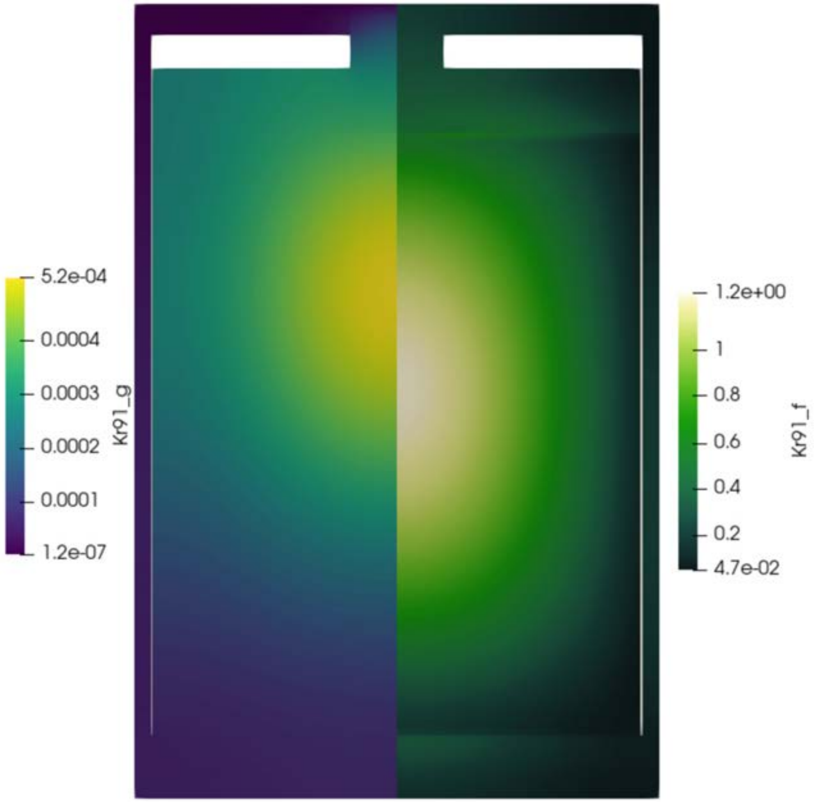
Fission: $y = 1.88654e - 4$

Fission: $y = 1.68E - 6$

Species Tracking: Steady-State Simulation Results 1/3

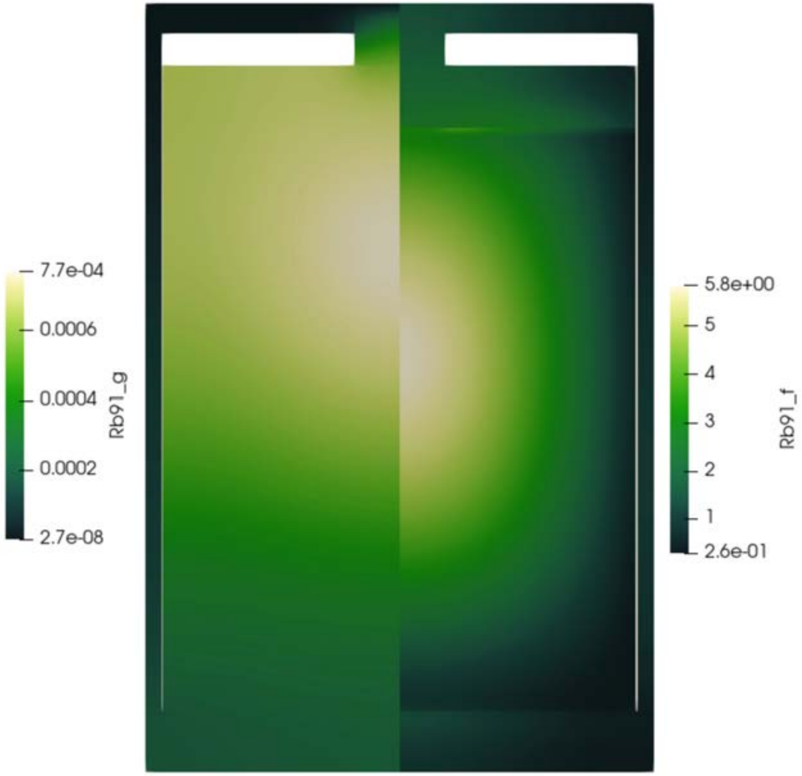
- ^{91}Br is produced by fission and stays in solution in the fuel salt
- No gaseous ^{91}Br is present
- ^{91}Kr is produced by fission and by natural decay of ^{91}Br in the fuel salt
- Some ^{91}Kr converts into the gas phase, where is transported toward the extraction point at the top of the reactor core

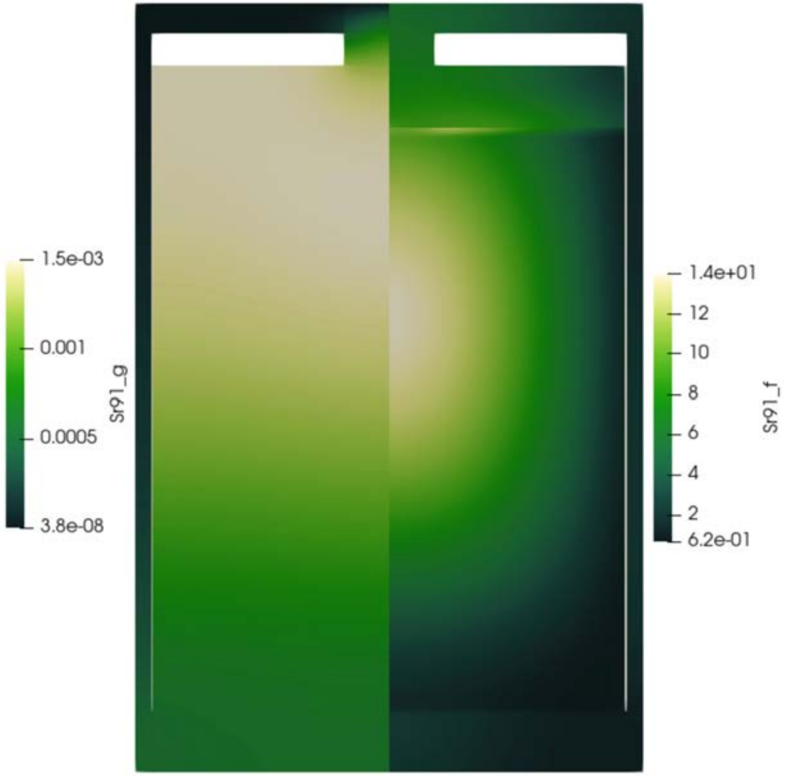




Species Tracking: Steady-State Simulation Results 2/3

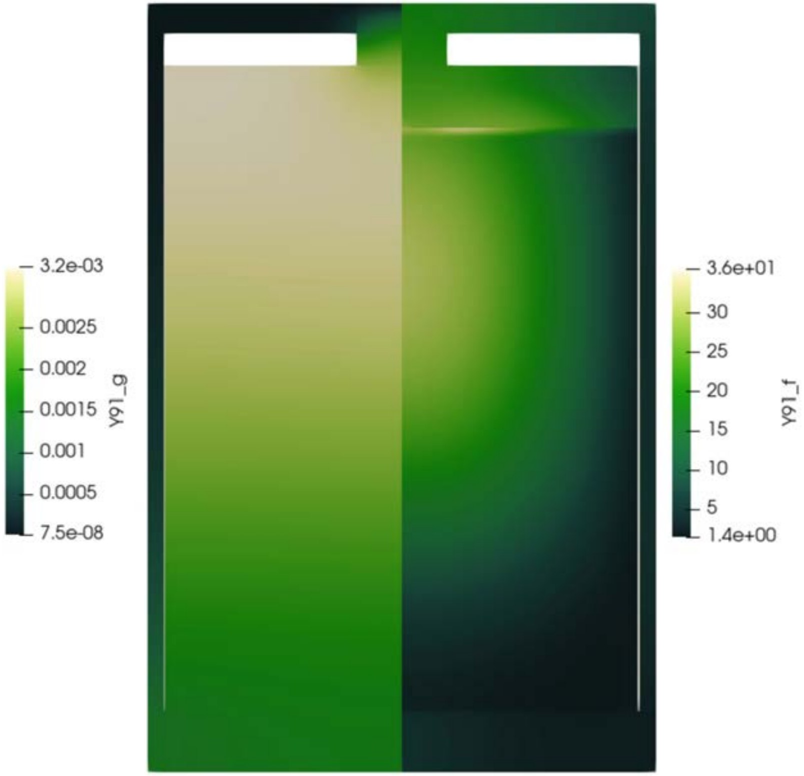
- ^{91}Rb is produced by fission and by the decay of ^{91}Kr in the fuel salt
- Also, ^{91}Rb is produced by the decay of ^{91}Kr in the gas phase
- A similar behavior is observed for ^{91}Sr

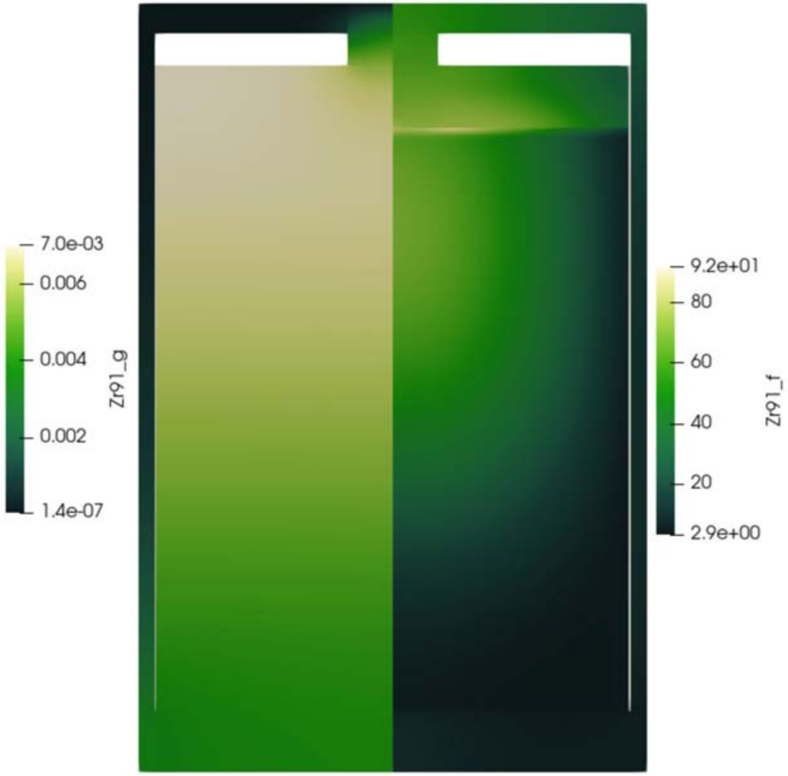




Species Tracking: Steady-State Simulation Results 3/3

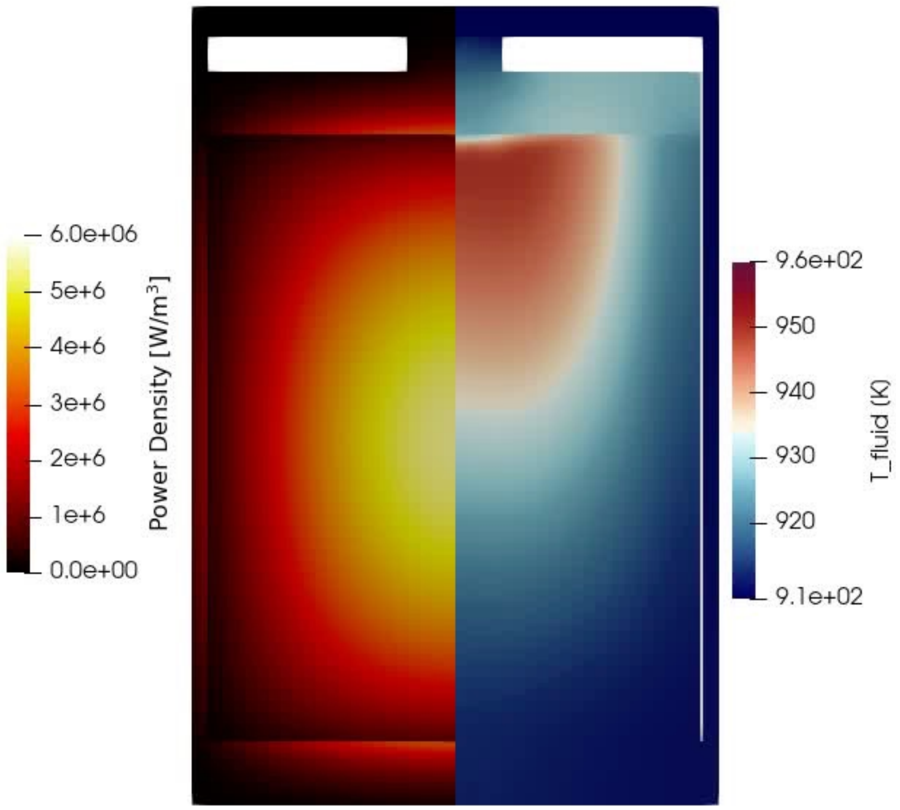
- ${}^{91}Y$ is produced by fission and by the decay of ${}^{91}Sr$ in the fuel salt
- There is no direct exchange between the liquid and the gas phase for ${}^{91}Y$
- Also, ${}^{91}Y$ is produced by the decay of ${}^{91}Sr$ in the gas phase
- A similar behavior is observed for ${}^{91}Zr$





MSRE – Reactivity Insertion Transient

- 100 pcms are injected in the reactor core at the initial time
- During a reactor transient, the distribution of void plays a fundamental role in power attenuation
- Additionally, the distribution of void is important in the reactor setpoint after the transient



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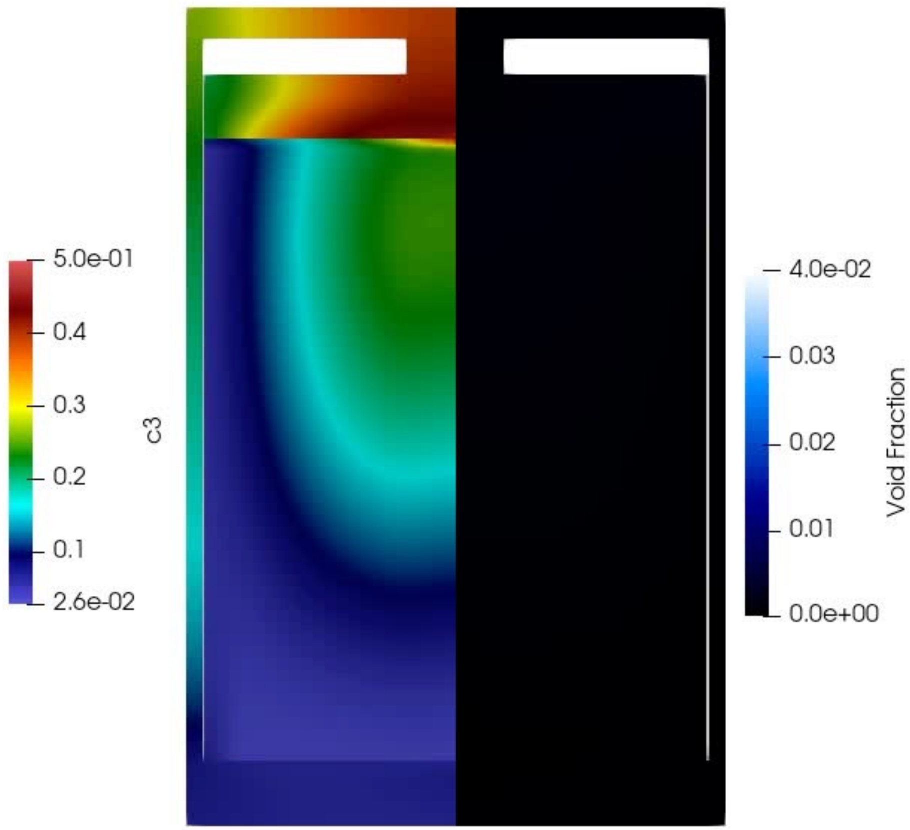

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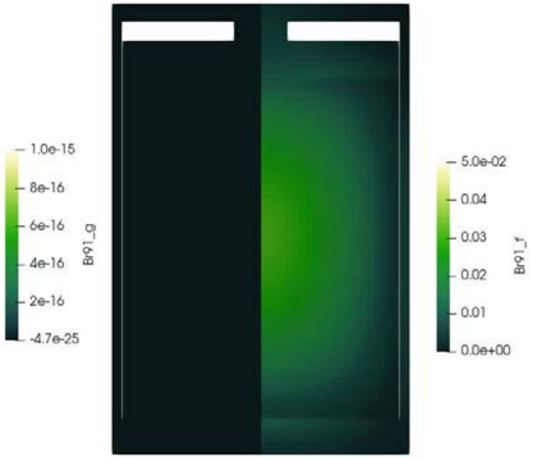
Evolution of species during reactivity insertion transient



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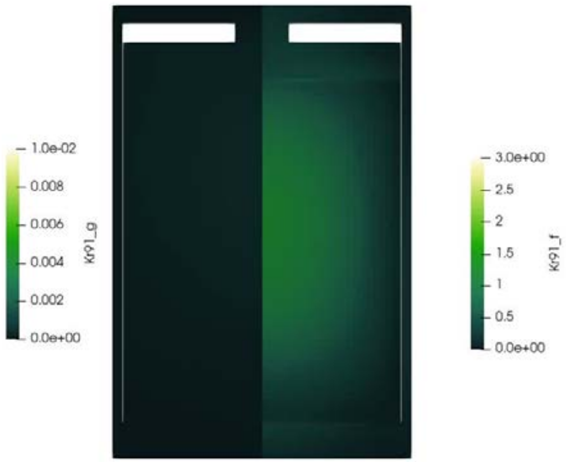

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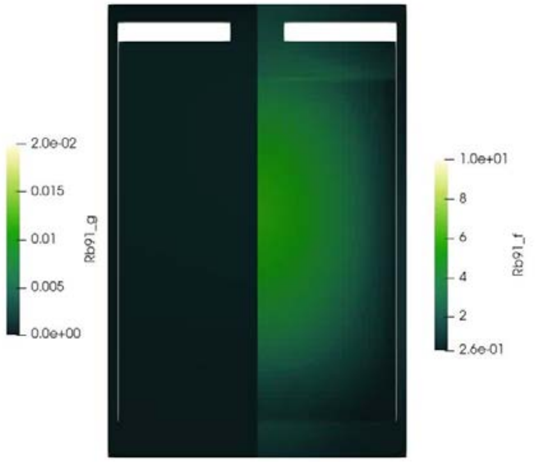

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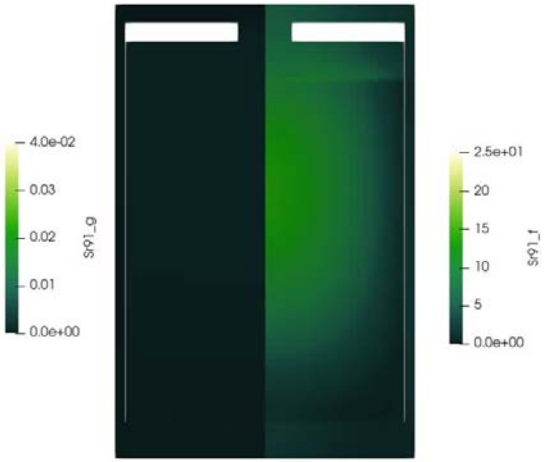

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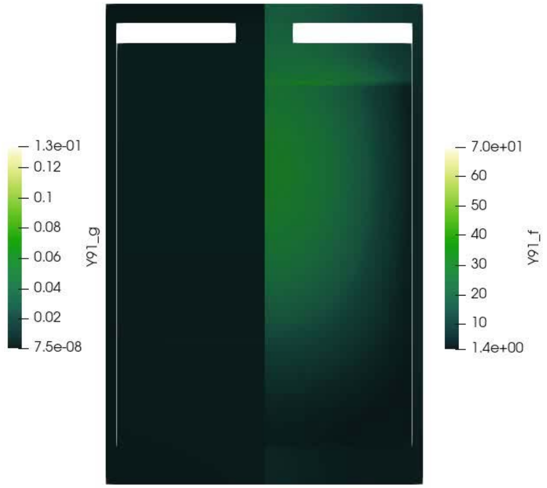

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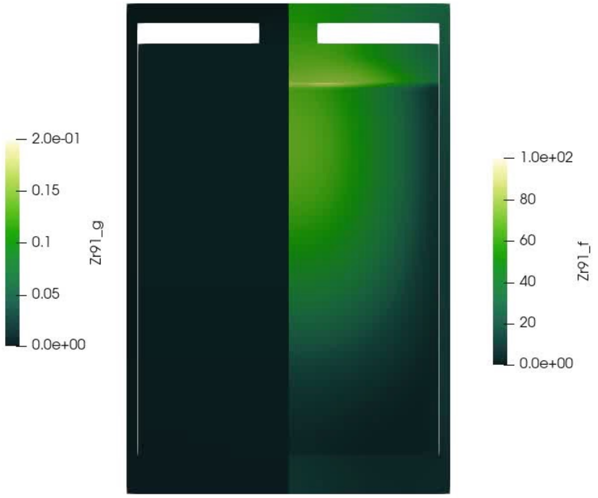

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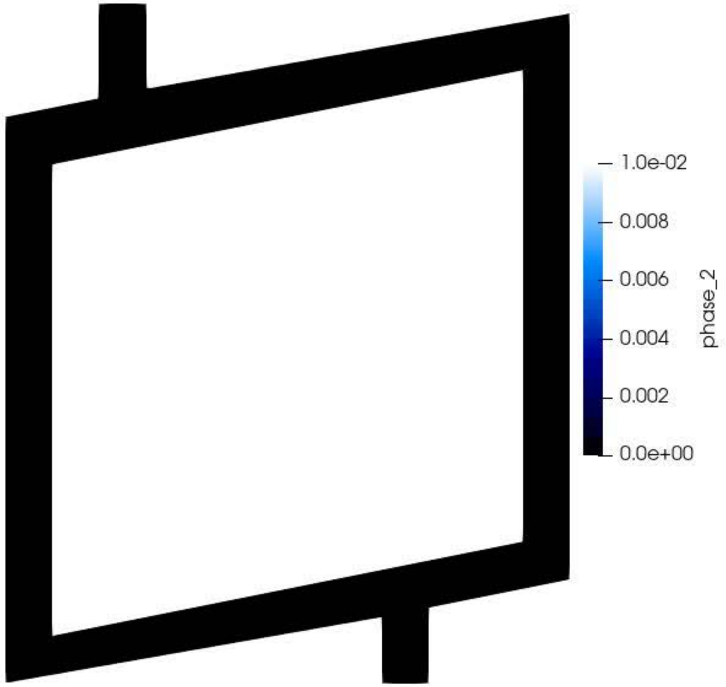
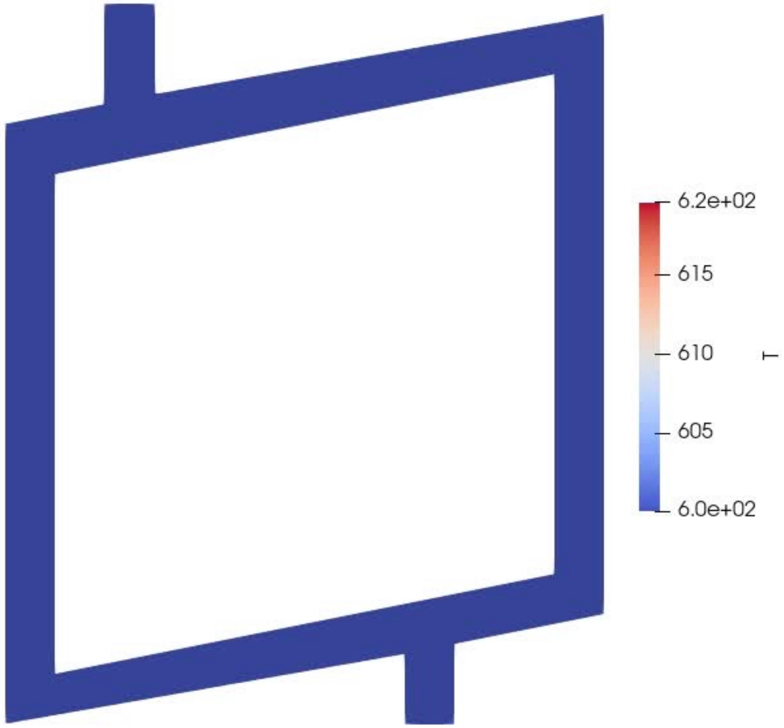
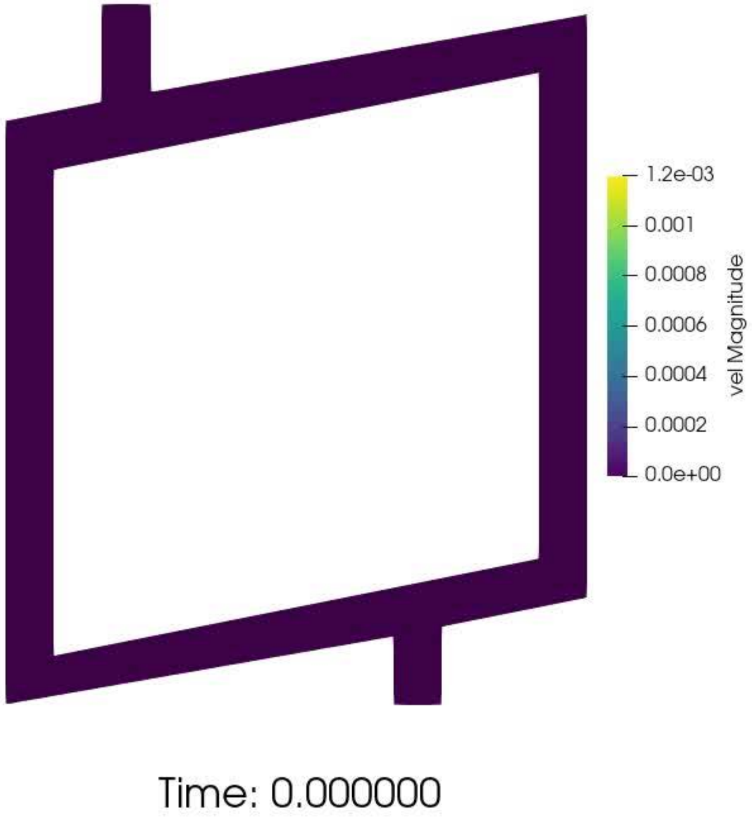
Experimental Testing

- Modeling Texas A&M experiment for Ar bubbles injected into natural-convection-driven FLiNaK loop
- Goal is determining the accuracy of out model in capturing Ar distribution throughout the loop







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Conclusions and Future Work

- **Key conclusions:**
  - New framework for coupled soluble + gaseous species tracking has been implemented using NEAMS tools
  - The model has been implemented for MSRE and shows the importance of modeling transients for accurate species tracking
- **Ongoing work:**
  - Validation of model results against MSRE composition measurements in salt samples and offgas system
  - However, this data is limited. We are seeking further experiment collaboration for model validation

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Thank you

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