MOSCATO Development and Validation

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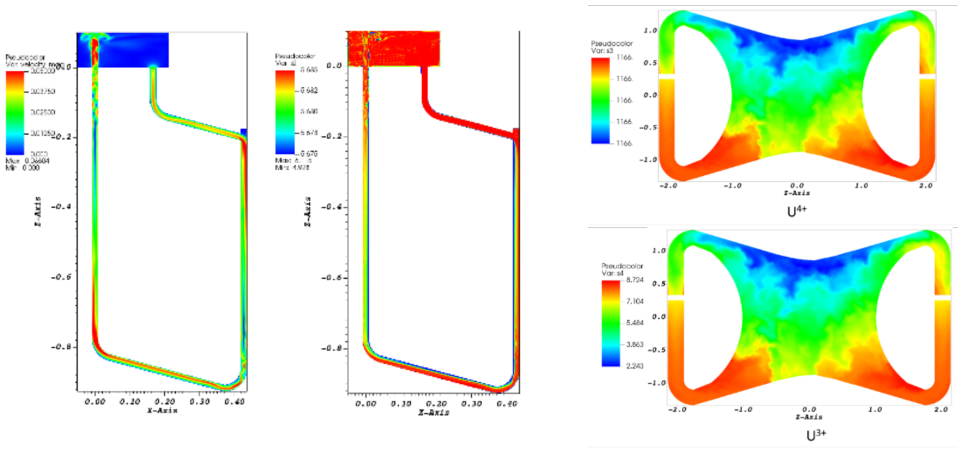
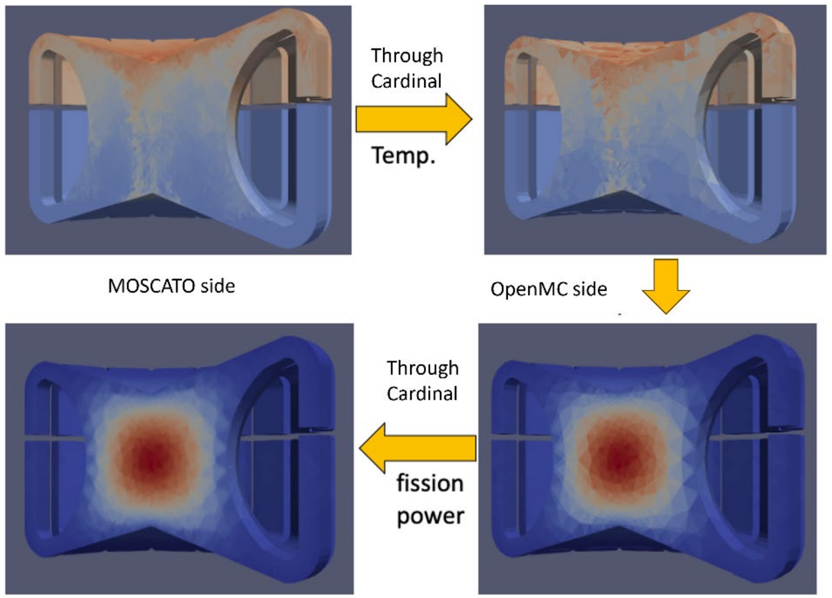
NEAMS

MOSCATO Overview

- What is MOSCATO ?
  - *MOlten Salt Chemistry And TranspOrt (MOSCATO)*
- An add-on to Nek5000/NekRS
  - Nek5000, the open-source Spectral Element Method CFD solver
  - NekRS, a refabricated version for GPU, orders faster than Nek5000
  - high-fidelity fluid-thermal solver (LES/DNS level)
- What is new?
  - Chemistry and electrochemistry phenomena
  - Structure corrosion simulations
  - Coupled neutronics
- Part of the NEAMS project for MSR applications



Cr^{2+} concentrations in typical TCL geometry (left), and contours of UF_x concentrations (right)



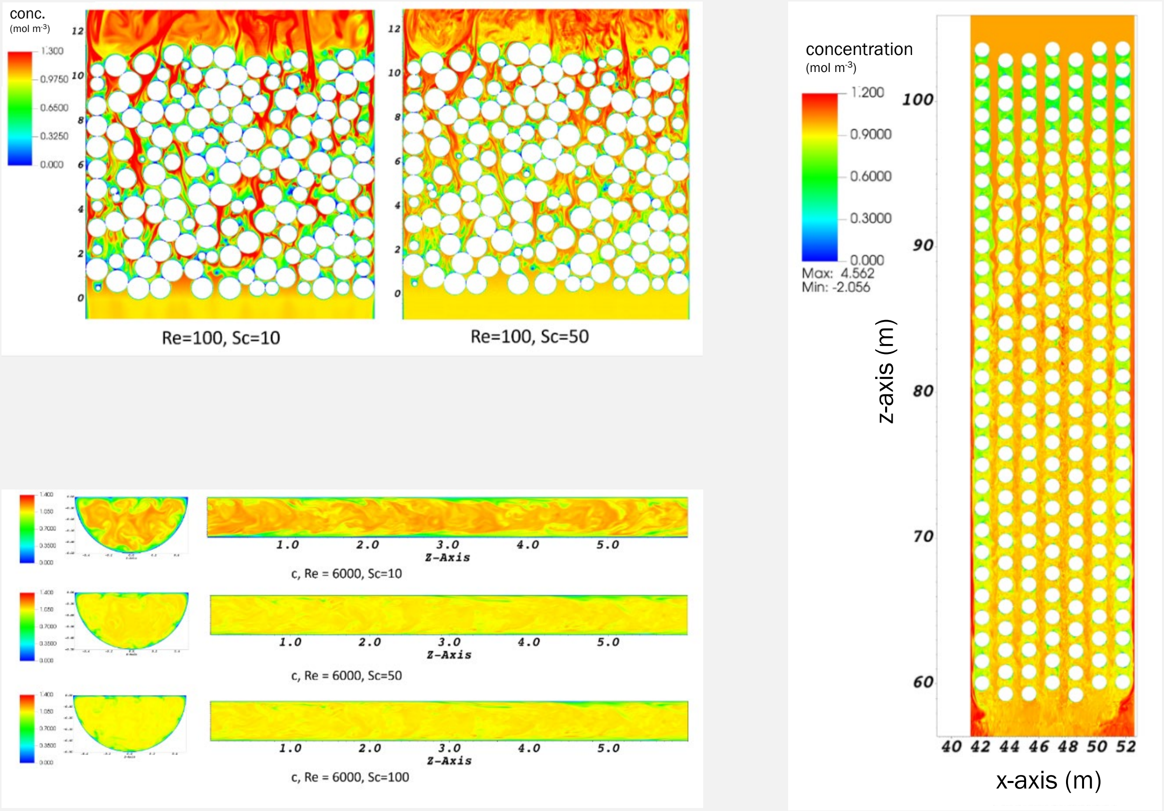
MOSCATO coupled with OpenMC through Cardinal

MOSCATO Overview

- **Benefits of using Nek5000/NekRS**
  - High-fidelity CFD (LES/DNS)
  - Same accuracy with less DOFs, or same DOFs but higher accuracy
  - High performance computing with high efficiency and strong scaling
  - Reduced computational source with GPU acceleration

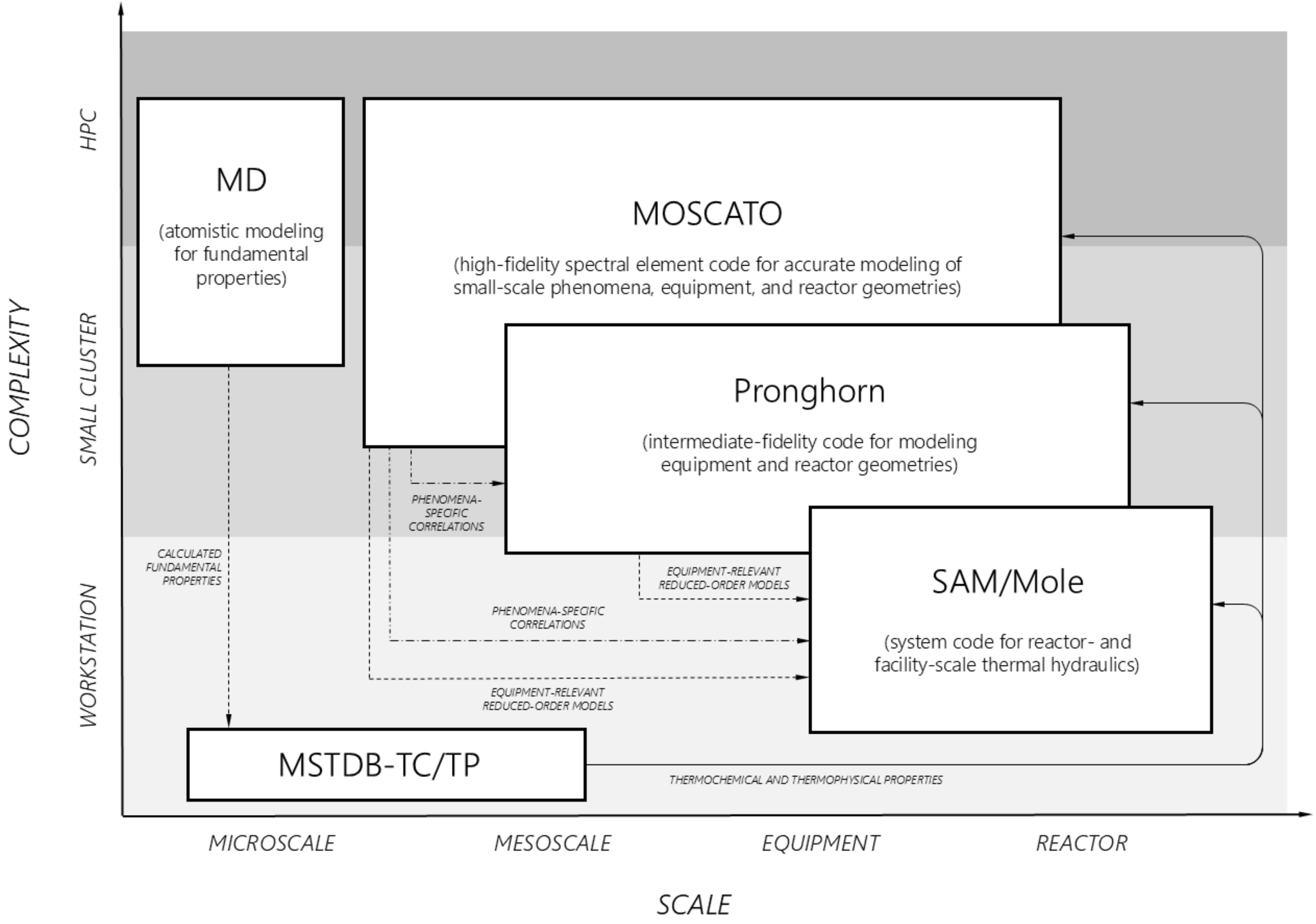
- **Benefits of using MOSCATO**
  - High-fidelity mass transport simulations
  - Complete electrochemistry solver
  - Structural corrosion simulator
  - Coupling to other NEAMS tool (SAM, Pronghorn, MOOSE, etc.)

High-Fidelity Simulations in Support of Reduced-Order Correlations



Mass transfer simulations for pebble bed and heat exchanger geometries

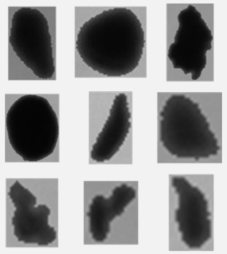
NEAMS MSR Chemistry/Corrosion Toolset

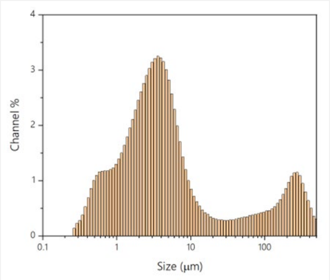


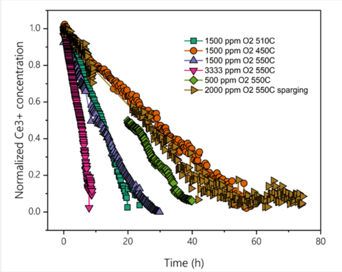
Recent Developmental Activities for MOSCATO

Phenomena of Interest

- Fission Gas Transport
- Effects from Gas Ingressions
- Particle Formation
- Noble Metal Deposition
- Gas/Liquid Mass Transport
- Corrosion Pathways

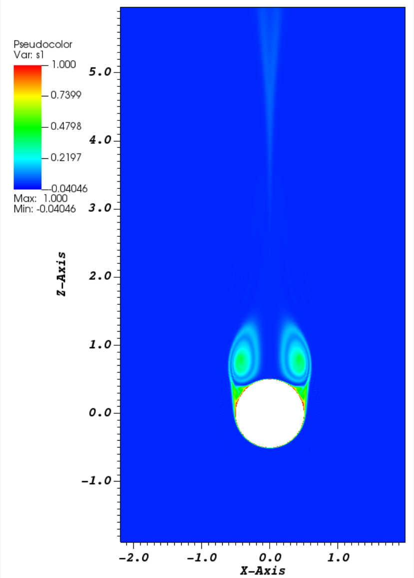


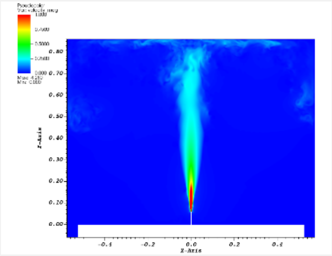


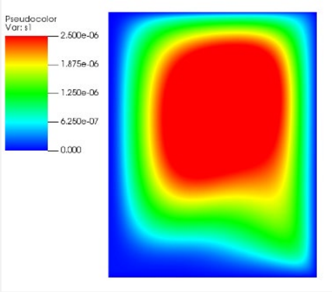


Targeted Modeling Developments

- Level-Set Method Implementation and V&V
- Eulerian-Eulerian Implementation and V&V
- Coupled Multiphase Flow with Chemistry
- Coupling to other NEAMS tool (SAM, MOOSE, etc.)







Multiphase Modeling: Level-Set Method

For helium bubble and gas ingression scenarios, full multiphase flow treatments must be implemented.

Level-set approaches have been adopted as they can be readily integrated into the Nek/MOSCATO framework to resolve phase interface.

- Transport equation of CLS (Conservative level-set)

$$\frac{\partial \psi}{\partial t} + \mathbf{v} \cdot \nabla \psi = S_{vv}(\psi)$$

- Re-initialization equation equation of CLS to maintain interface

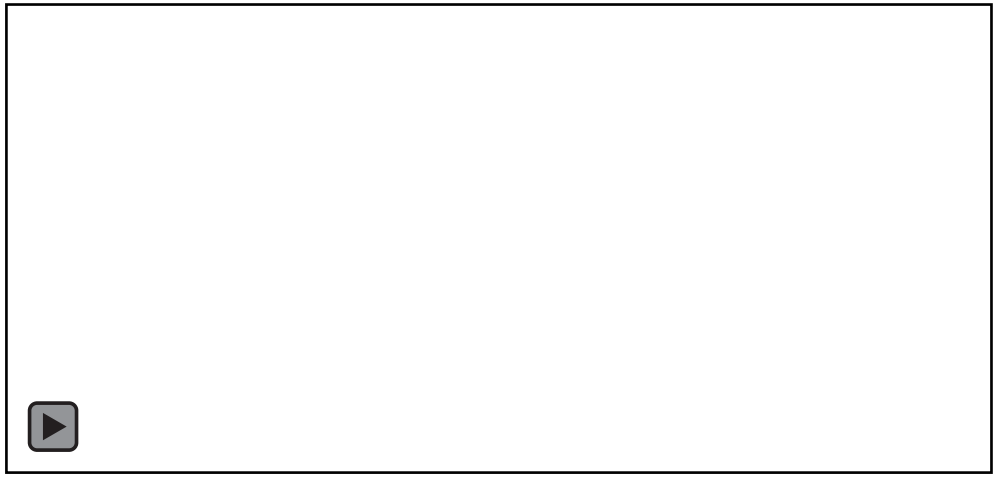
$$\frac{\partial \psi}{\partial \tau} + \nabla \cdot (\psi(1-\psi)\mathbf{n}) = \nabla \cdot (\epsilon(\nabla \psi \cdot \mathbf{n})\mathbf{n}) + S_{vv}(\psi)$$

Verification performed with respect to reference numerical data

Validation underway comparing results to helium bubble evolution in molten salt

Reference numerical data (Re=70, We = 20)[1]

MOSCATO results (Re=70, We = 20)

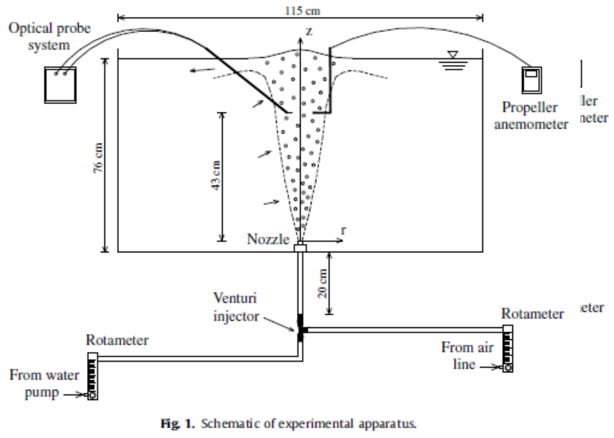


MOSCATO simulation of bubble rise

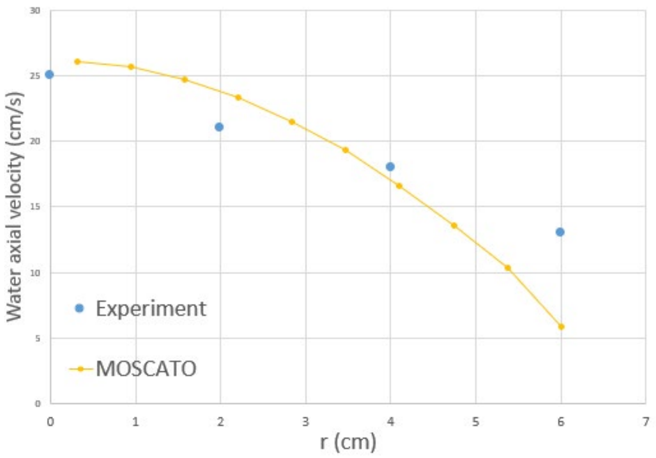
[1]Nat. Comm, 17, 6(1):6268 2015

Mixture Model Implementation for Gas/Liquid Systems

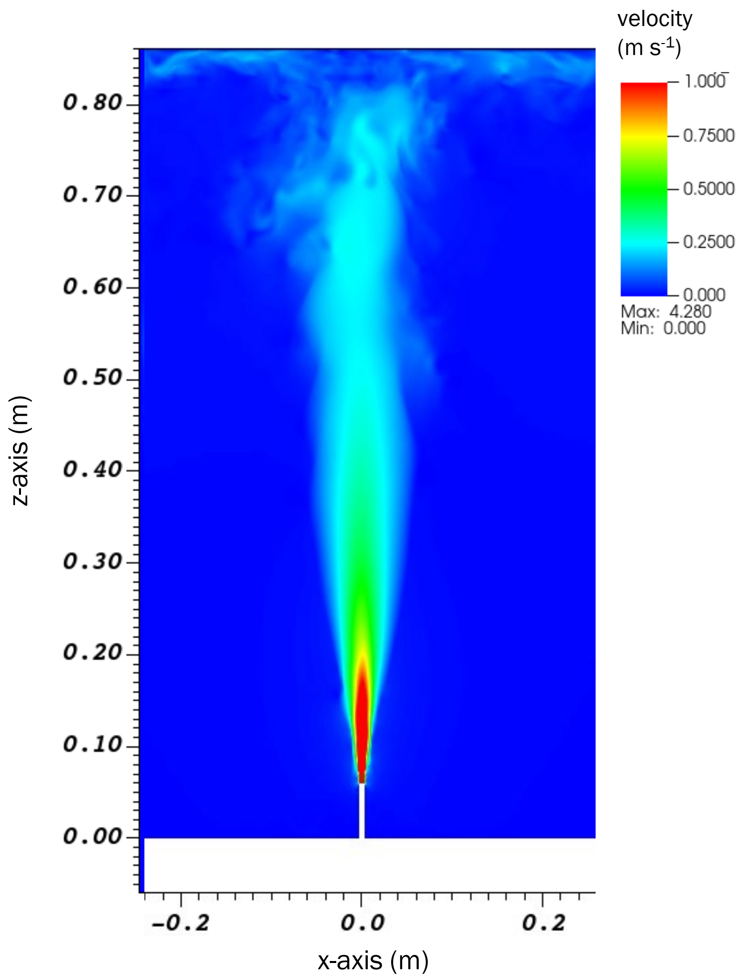
- When bubble numbers are large (e.g., for sparged systems) explicitly resolving bubbles become numerically expensive and infeasible
- Mixture Model Implementation
    - Solving mixture momentum equation
    - Solving relative velocity with algebraic model
        - Many interphase momentum transfer options available
        - Work in progress to refine models and parameters
- Validation of the mixture model being performed for bubbly flow jet experimental data in water
    - Planned validation using O_2/H_2O sparging data from DOE MRWFD program



Experiment setup (bubbly flow jet in water)[1]



Liquid velocity profile at sampling location



Liquid velocity profile with RANS model (k-tau)

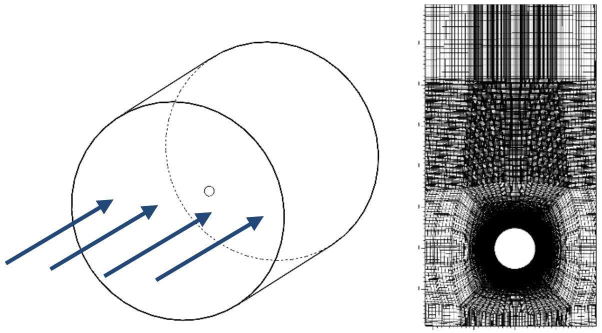
[1]Neto, Iran E. Lima, David Z. Zhu, and Nallamuthu Rajaratnam. "Bubbly jets in stagnant water." International Journal of Multiphase Flow 34, no. 12 (2008): 1130-1141.

Results: High Schmidt Number Mass Transfer to Bubble Interfaces

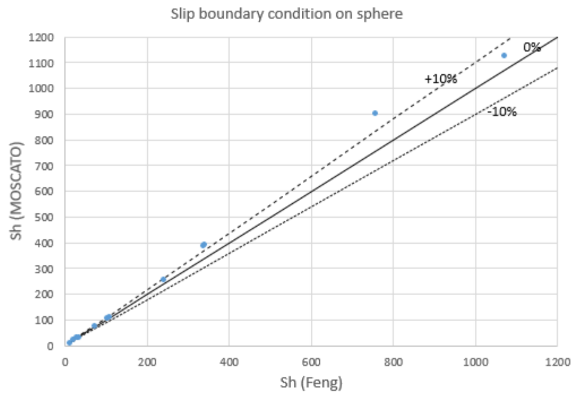
- Modeling of mass transfer of dissolved species to and from salt/gas/solid interfaces is essential
    - Transport to interface often controls reaction rates

- Objective:
    - Improve current Sherwood number correlation across relevant ranges of Reynolds and Schmidt numbers, targeting for high Sc numbers, for bubble interface
    - *Re* (1-10000), *Sc* (1-100)

- Improved correlations have been provided to other partners labs within the MSR Chemistry/Corrosion thrust

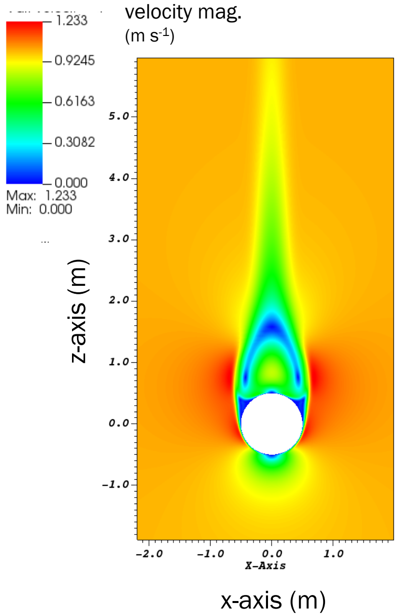


Computational domain and mesh

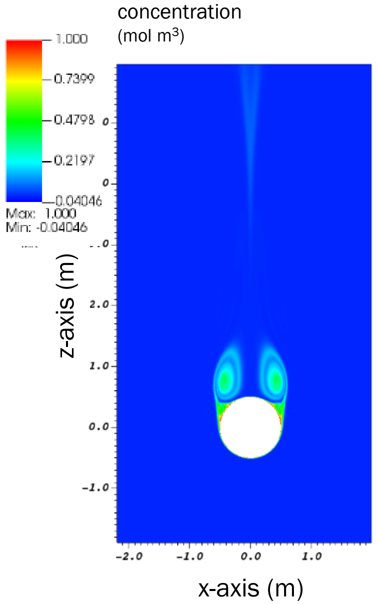


$$Sh = 0.651\,Re^{1/2}Sc^{1/2}\left(1.032 + \frac{0.61\,Re}{Re+21}\right) + \left(1.60 + \frac{0.61\,Re}{Re+21}\right)$$

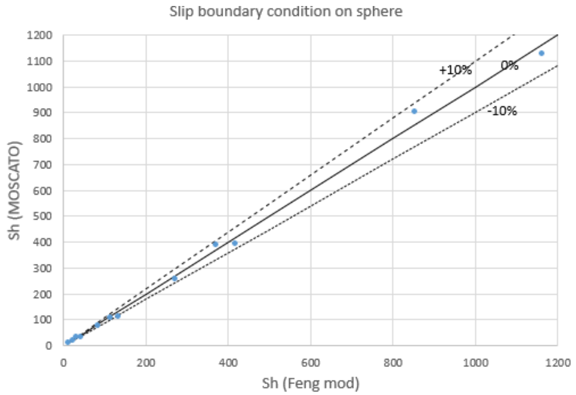
Mass transfer correlation from reference



Velocity contours around gas bubble



Concentration contours around gas bubble



$$Sh = 0.935\,Re^{0.497}Sc^{0.445}\left(1.032 + \frac{0.61\,Re}{Re+21}\right) + \left(1.60 + \frac{0.61\,Re}{Re+21}\right)$$

Improved mass transfer correlation

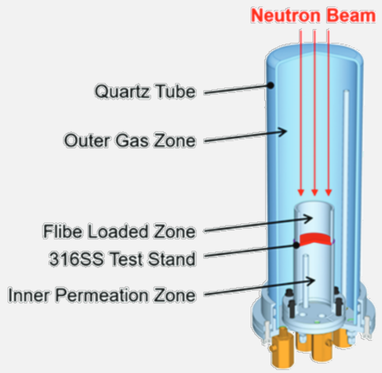
Results: Dissolved Tritium Transport Simulations

Capabilities for modeling dissolved tritium transport within the salt and structural alloys has been implemented

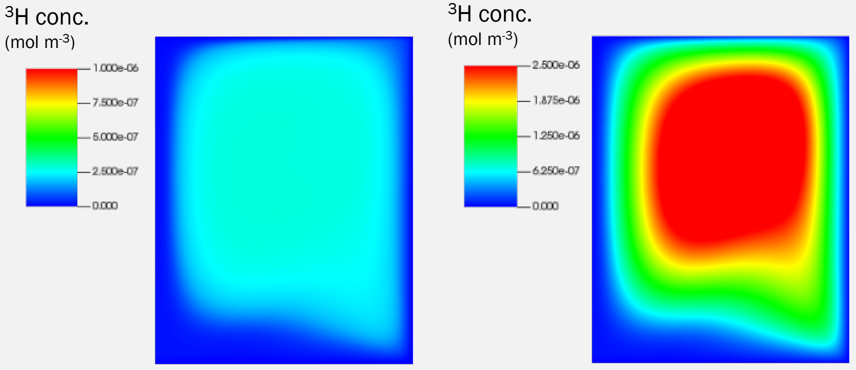
- Proper modeling of tritium transport is essential within many MSRs as it is generated by neutron activation of Li

- MOSCATO can accurately predict the transport of tritium within the coupled salt/alloy system
  - Tritium release rate through permeation zone matches experimental data
  - Natural circulation induced by temperature differences also accurately predicted

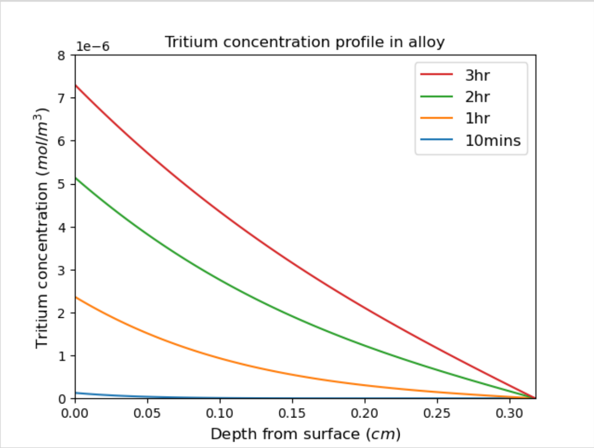
Tritium Transport Validation Case



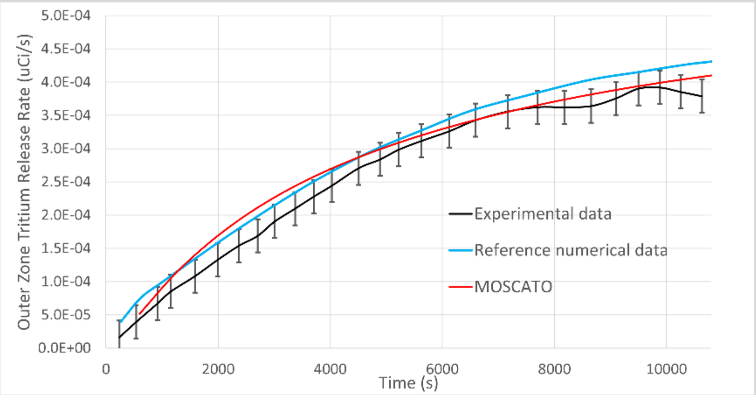
Neutron irradiated FLiBe in capsule with off-gas measurements[1]



2D axisymmetric tritium concentration in salt (10 mins and 3 hr)



Tritium concentration within alloy



Tritium release rate time history

[1]Dolan, et al., Nuc Tech 2023

Results: Molten Salt Corrosion Validation

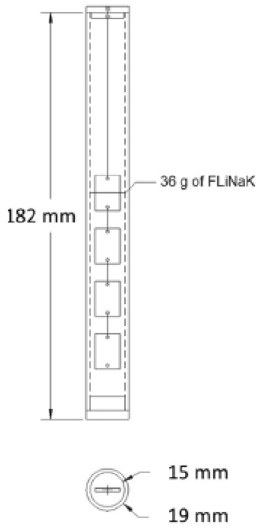
- Additional validation of corrosion modeling was performed in FY24 for static and flowing cases
- Static cases examined include corrosion experiments conducted at UW-Madison[1]
  - Stainless steel sample in static salt at high temperature (700 °C)
  - Added impurity in the salt to accelerate corrosion.
- Cases include moisture and multiple corrosion products

Corrosion Mechanisms

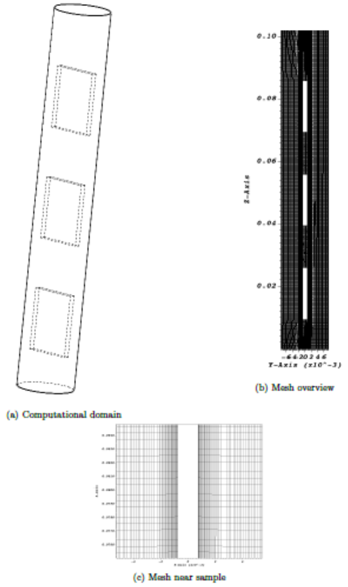
$$Cr^{2+} + 2e^{-} \leftrightarrow Cr$$

$$Fe^{2+} + 2e^{-} \leftrightarrow Fe$$

$$2H^{+} + 2e^{-} \leftrightarrow H_2$$



Experimental apparatus[1]



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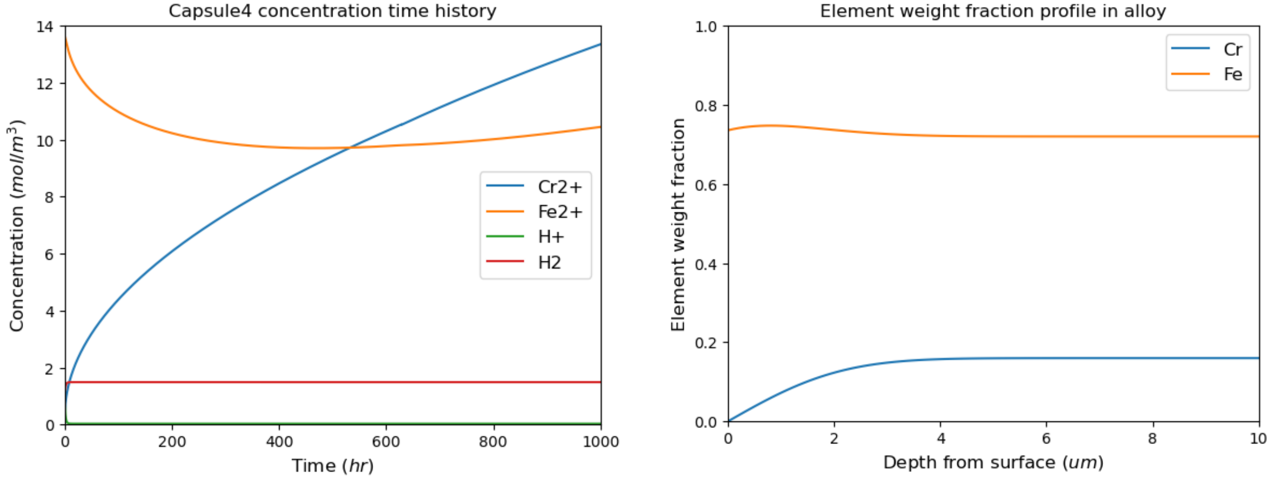

Evolution of corrosion product concentrations in capsule over time (left) and alloy composition as function of distance from interface (right)

Case	Exp m_l or m_c (mg/cm^2)	MOSCATO m_l (mg/cm^2)
Capsule 1	0.26 ± 0.05	0.22
Capsule 2	0.198 ± 0.004	0.215
Capsule 3	0.22 ± 0.07	0.21
Capsule 4	0.24 ± 0.04	0.18

Experiments and simulated results from MOSCATO show good agreement

[1]Doniger, William H., Cody Falconer, Mohamed Elbakhshwan, Karl Britsch, Adrien Couet, and Kumar Sridharan. "Investigation of impurity driven corrosion behavior in molten 2LiF-BeF2 salt." Corrosion Science 174 (2020): 108823.

Summary

- Additional modeling capabilities have been added to MOSCATO in FY25 to further expand the applicability of its high-fidelity CFD-level multiphysics simulations for MSR applications
  - Improved electrochemistry solver
  - Updated Structural corrosion simulator
  - Tritium transport solver
  - Bubbly flow solver
  - Level-set capabilities

- Due to its high-fidelity, scalable multiphysics feature set, MOSCATO can solve problems from small-scales up through component, loop, and reactor level simulations

Future Work

- Continued implementation of combined multiphase flow / chemistry solvers
  - Validation to experimental O_2/H_2O ingression testing
  - Inclusion of particle generation
- Implementation of gas phase reactions
- Continued simulations of reactor-relevant geometries
  - Generation of low-order correlations for system-level tools
- Full-scale reactor simulations

Acknowledgements

Funding Acknowledgement

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