Reactive Multiphase Flow Modeling with MOSCATO

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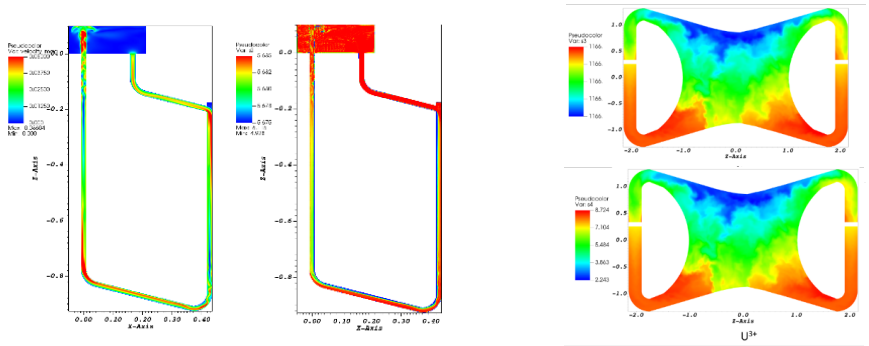
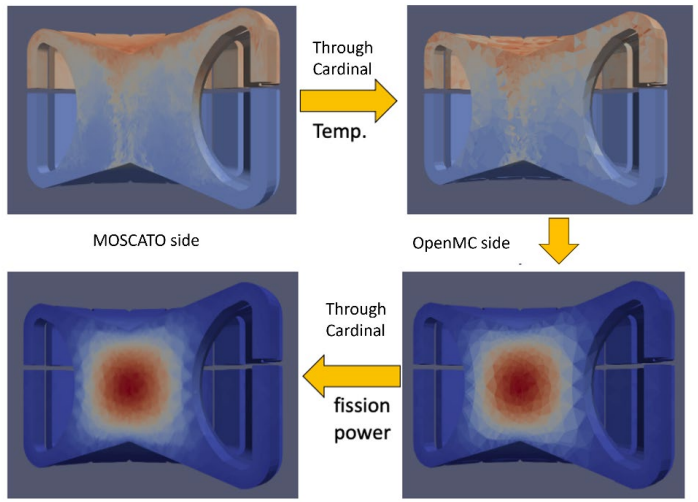
MOSCATO Overview

Full-Scale Thermal Convection Loop and Reactor Core Simulations

- What is MOSCATO ?
  - ***MO**lten **S**alt **C**hemistry **A**nd **T**ransp**O**rt (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) for HPC
- What is new?
  - Chemistry and electrochemistry phenomena
  - Structure corrosion simulations
  - Coupled neutronics
  - *Multiphase Reactive Transport*



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

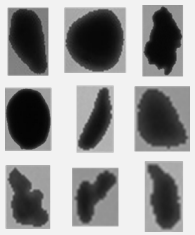


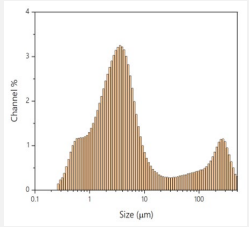
MOSCATO coupled with OpenMC through Cardinal

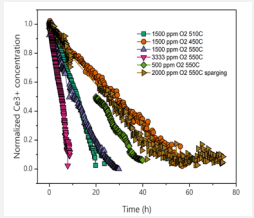
Recent Developmental Activities for MOSCATO

Additional Phenomena of Interest

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

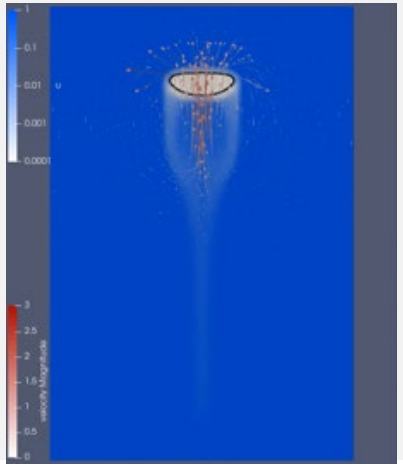


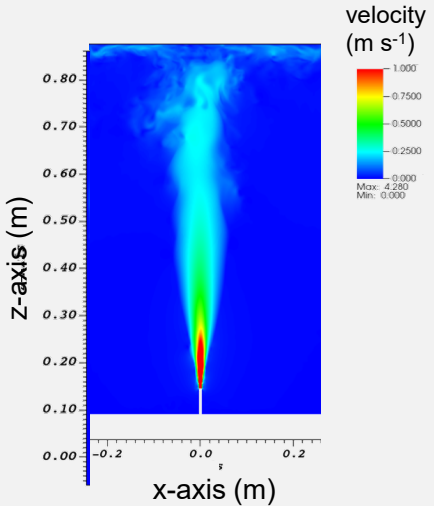




Recent Modeling Developments

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





Multiphase Modeling: *Level-Set Method*

Level-set methods have been implemented in the Nek/MOSCATO framework to enable modeling of fission gas bubble and gas ingression scenarios

- Higher-order numerical method to capture interface between two phases.
- Novel level-set method for incompressible two-phase flows in the continuous Galerkin (CG) high order spectral element framework

MOSCATO's level-set implementation has been validated for various applications such as:

- Rayleigh-Taylor Instability
- Dam break problem
- Single-bubble rising in molten salt (experiment by Chavez et al at TAMU)
  - Salt: FLiNaK; Gas: helium; System temperature: 575 C

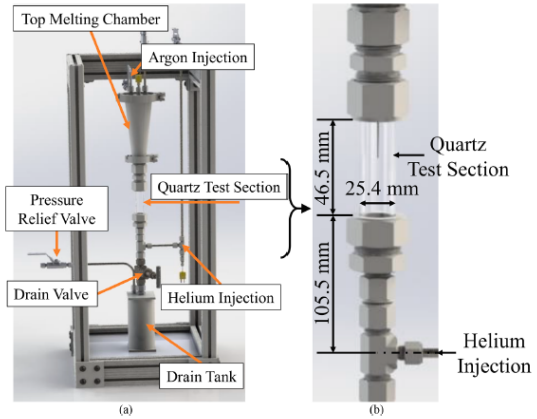
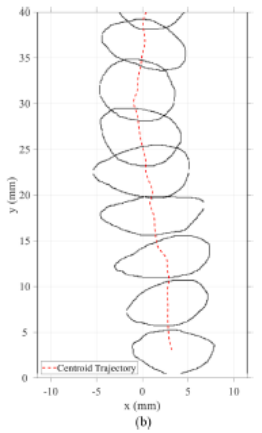


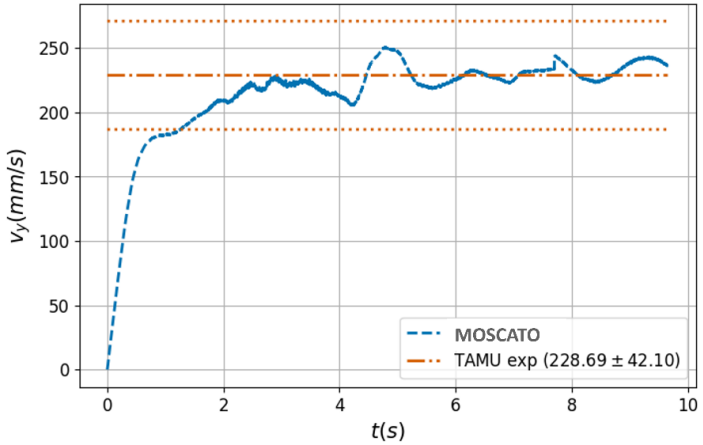
Fig. 1. (a) Overview of the test system. (b) Close up of clear test section with dimensions.

Experiment facility [1]



Experiment bubble trajectory [1]

MOSCATO bubble trajectory



Predicted and experimental bubble velocity

[1] D. E. Chavez, S. R. Yang, R. Vaghetto, and Y. A. Hassan, "Experimental investigation of single helium bubbles rising in FLiNaK molten salt," International Journal of Heat and Fluid Flow, 92, pp. 108875 (2021)

Multiphase Modeling with Mass Transport

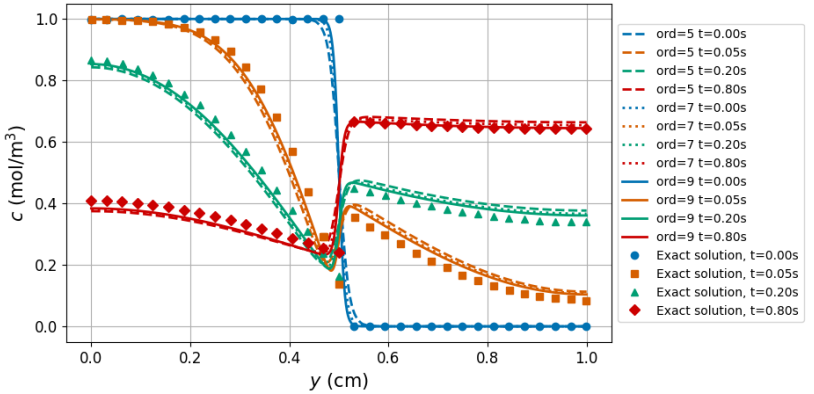
Mass transport was integrated into MOSCATO's level-set model.

- New functionality enables simulation of transport of dissolved gases to and from gas-liquid interface
- Model has been validated against 1-D analytical solution for oxygen transfer between water and air.

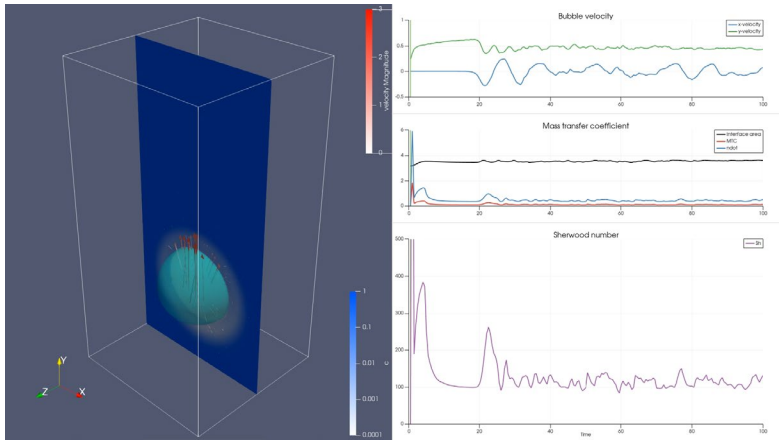
$$\frac{\partial c}{\partial t} = -\nabla \cdot (c\vec{u}) + \nabla \cdot \left(\frac{D_1 \alpha H + D_2(1-\alpha)}{\alpha H + (1-\alpha)} \nabla c \right) - \nabla \cdot \left(\frac{H D_1 - D_2}{\alpha H + (1-\alpha)} c \nabla \alpha \right)$$

Three-dimensional single bubble simulations have also been performed demonstrating the capability to model bubble growth

- Conservative mass sink and sources included inside bubble and salt regions
- Mass transfer across evolving bubble is recorded
- Parameters: Re = 511.9, We = 1.446, Sc = 453.1



Concentration profiles during mass exchange through gas/liquid interface [1]

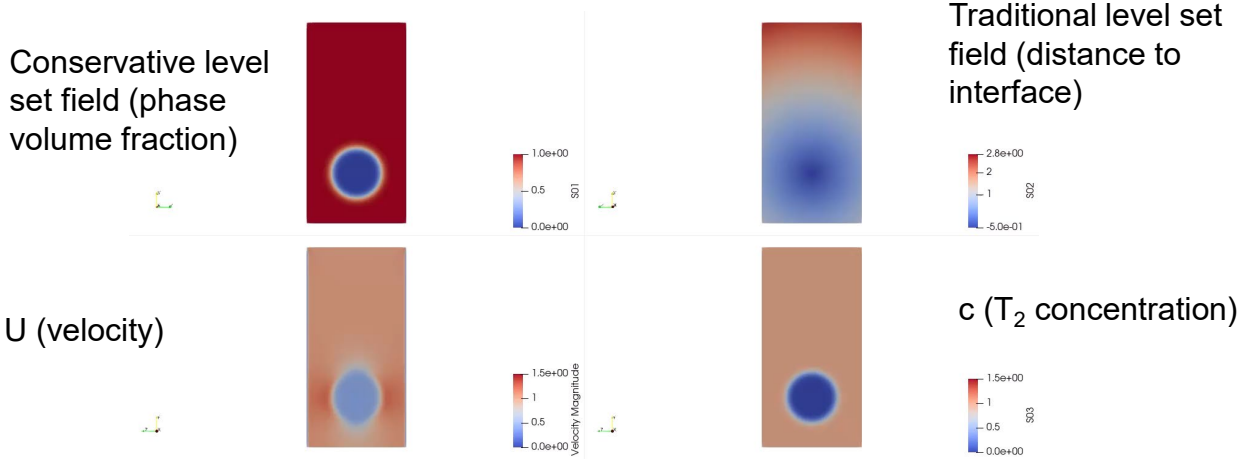


MOSCATO single bubble dynamics with mass transfer

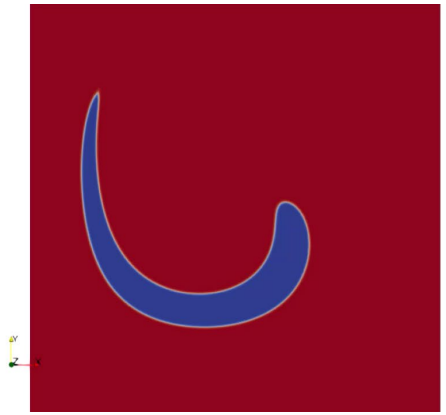
[1] Marschall, H., Hinterberger, K., Schüler, C., Habla, F., & Hinrichsen, O. (2012). Numerical simulation of species transfer across fluid interfaces in free-surface flows using OpenFOAM. *Chemical engineering science*, *78*, 111-127.

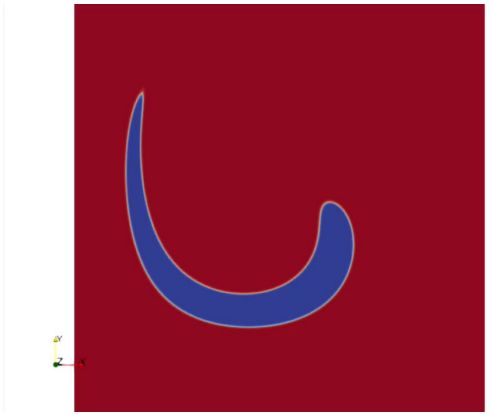
Multiphase Modeling with Mass Transport

- Previous implementation was done in Nek5000 (CPU version).
- We are currently migrating the level set capability to NekRS (GPU version)
  - A significant acceleration is observed with GPU (10×)
  - In parallel we are also implementing species transport model in GPU version, but with unmoving interface



Mass transfer through bubble interface





NekRS, 4 GPUs
1.4 M GLL per GPU
Total solve time: 377s

Nek5000, 400 procs
14k GLL/proc (40 E/proc)
Total solve time: 3317s

Rider-Kothe Vortex [1][2]

[1] Saini, N., Shaver, D., Tomboulides, A., Obabko, A., & Merzari, E. (2025). *Spectrally Stabilized Interface Capturing Formulation and Implementation in Nek5000/NekRS* (No. ANL/NSE--25/51). Argonne National Laboratory (ANL), Argonne, IL (United States).
[2] Kumar, R., Cheng, L., Xie, B., & Xiao, F. (2019). THINC-scaling scheme that unifies VOF and level set methods. *arXiv preprint arXiv:1908.04529*.

Bubbly flow solver for Multiphase Modeling

- When their numbers are large, explicitly resolving individual bubbles becomes numerically expensive and infeasible

- Mixture Model Implementation
  - Semi Eulerian–Eulerian approach solves void fraction, relative velocity, etc.
  - Assumes small bubbles/particles that reach momentum equilibrium instantaneously

- MOSCATO's implementation is applicable to:
  - Sparged systems
  - Fission gas transport
  - Distillation equipment
  - Transport of micro- to milli-scale particles

$$\frac{\partial \alpha}{\partial t} + \mathbf{u}_m \cdot \nabla \alpha = -\alpha \nabla \cdot \mathbf{u}_m - \nabla \cdot (\alpha \mathbf{u}_{dr}) + \nabla \cdot \left(\frac{\nu_t}{Sc_t} \nabla \alpha \right) + \gamma$$

Equation for void fraction

$$\rho_g \frac{d\mathbf{u}_g}{dt} = \Delta \rho g - \frac{3}{4 d_p} C_D \rho_l \mathbf{u}_{re} \left| \mathbf{u}_{re} \right| - C_{TD} \rho_l k \nabla \alpha - C_L \rho_l \mathbf{u}_{re} \times (\nabla \times \mathbf{u}_l)$$

Equation for relative velocity

$$\frac{3}{4 d_p} C_D \rho_l \mathbf{u}_{re} \left| \mathbf{u}_{re} \right| + C_L \rho_l \mathbf{u}_{re} \times \omega = \Delta \rho g - C_{TD} \rho_l k \nabla \alpha$$

$$\begin{bmatrix} \frac{3}{4 d_p} C_D \rho_l \left| \mathbf{u}_{re} \right| & \omega_z C_L \rho_l & -\omega_y C_L \rho_l \\ -\omega_z C_L \rho_l & \frac{3}{4 d_p} C_D \rho_l \left| \mathbf{u}_{re} \right| & \omega_x C_L \rho_l \\ \omega_y C_L \rho_l & -\omega_x C_L \rho_l & \frac{3}{4 d_p} C_D \rho_l \left| \mathbf{u}_{re} \right| \end{bmatrix} \cdot \begin{bmatrix} u_{re,x} \\ u_{re,y} \\ u_{re,z} \end{bmatrix} = \begin{bmatrix} \Delta \rho g_x - C_{TD} \rho_l k \frac{\partial \alpha}{\partial x} \\ \Delta \rho g_y - C_{TD} \rho_l k \frac{\partial \alpha}{\partial y} \\ \Delta \rho g_z - C_{TD} \rho_l k \frac{\partial \alpha}{\partial z} \end{bmatrix}$$

Simplified algebraic relationship for equilibrated small particles

Bubbly flow solver for Multiphase Modeling

- Validation of the mixture model has been performed using a variety of bubbly flow jet experimental data
  - Initial validation for multiphase flow solver using air/water systems
- Validation at present is fair; additional treatment of bubble lift force is likely needed to improve void fraction profiles
- Planned validation of combined chemistry solver using O_2/H_2O sparging data from DOE MRWFD program

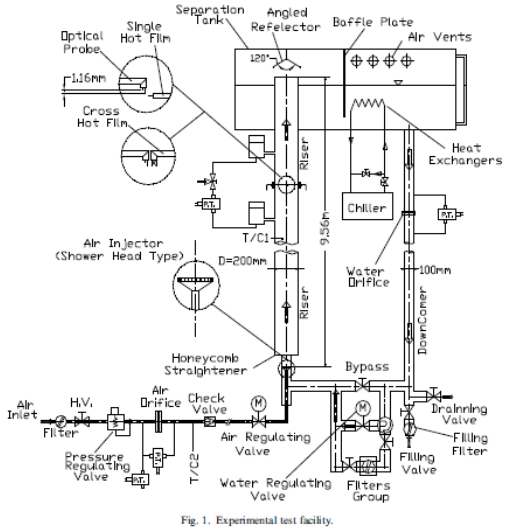
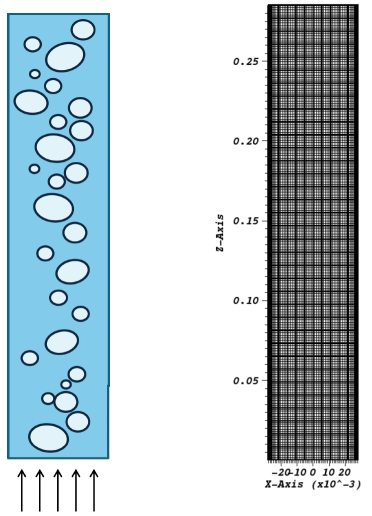
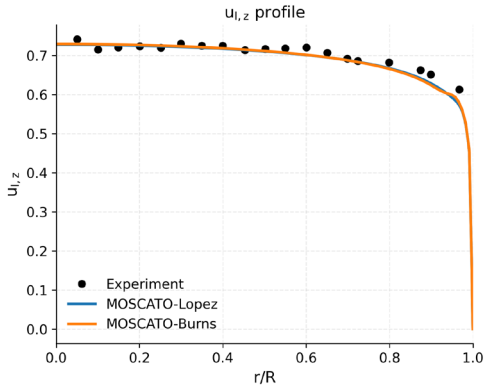


Fig. 1. Experimental test facility.

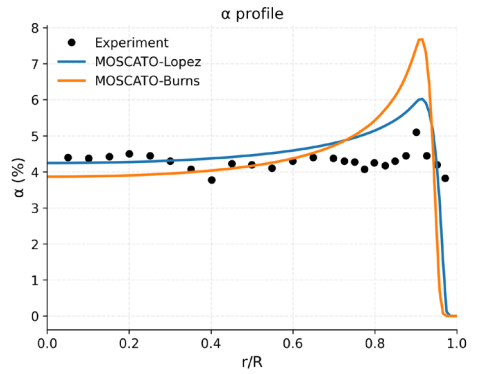
Experiment facility for water/air testing [1]



Computational domain and mesh



Liquid velocity profile



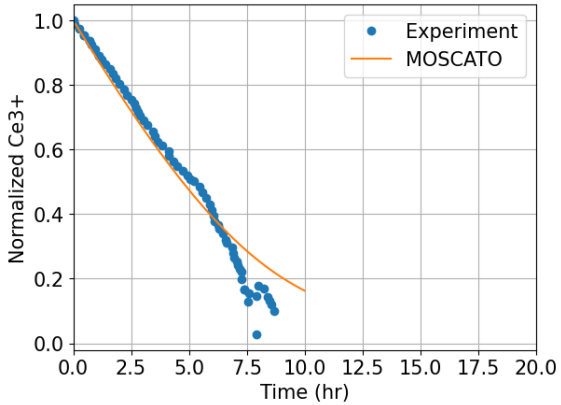
Void fraction profile

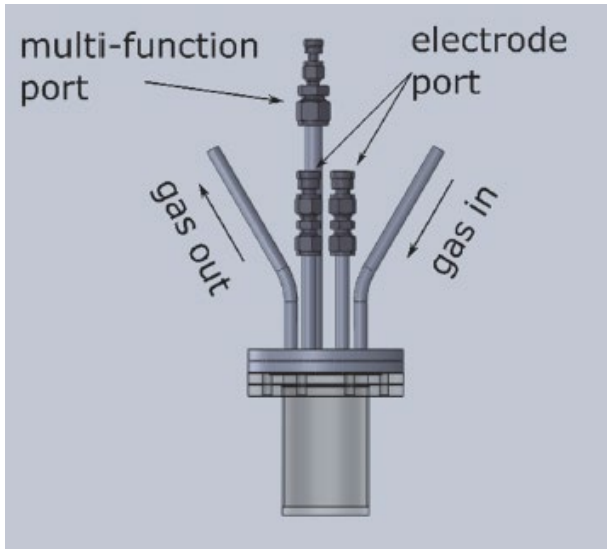
[1] M. Shawkat, C. Ching, and M. Shoukri, "Bubble and liquid turbulence characteristics ofbubbly flow in a large diameter vertical pipe," International Journal of Multiphase Flow, 34(8), pp. 767–785 (2008)

Oxygen ingressions into molten salt

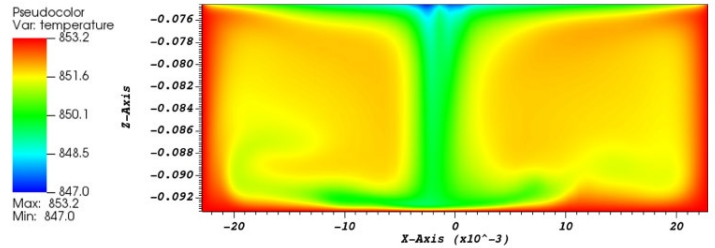
- Validation for reactive multiphase flow is being developed based on experimental oxygen and moisture ingression tests conducted at Argonne.
- $Ar/O_2/H_2O$ gas is injected into the vessel headspace or is sparged into the salt the salt (LiCl-KCl-$CeCl_3$).
  - Ingression gases enter the salt and react with $CeCl_3$ via a variety of mechanisms that can lead to the formation of CeO_2 or CeOCl .

Reaction
$CeCl_3 + 3H_2O \rightarrow Ce(OH)_3 + 3HCl$
$2Ce(OH)_3 \rightarrow 2CeO_2 + H_2 + 2H_2O$
$Ce(OH)_3 + HCl \rightarrow CeOCl + 2H_2O$
$CeCl_3 + H_2O \rightarrow CeOCl + 2HCl$
$2CeCl_3 + 4H_2O \rightarrow 2CeO_2 + 6HCl + H_2$

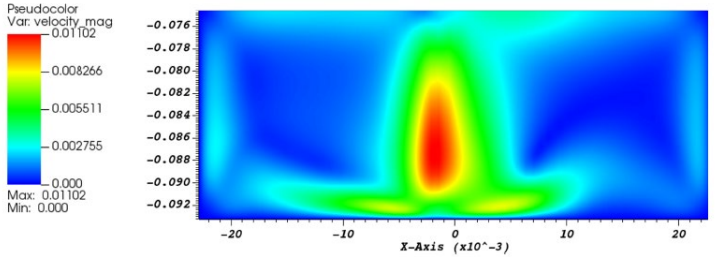




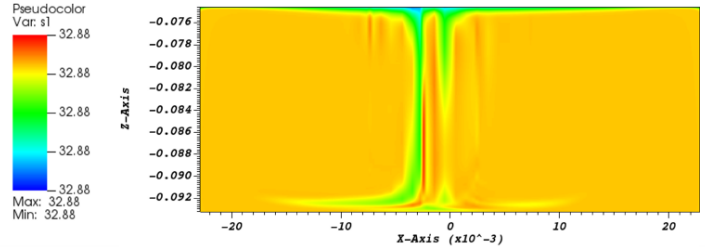
Reaction vessel for oxygen ingression tests [1]



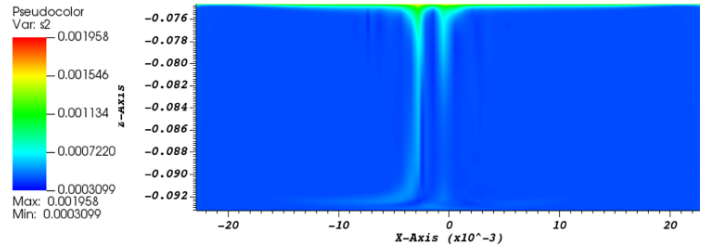
(a) Temperature



(b) Velocity magnitude



(a) Ce3+



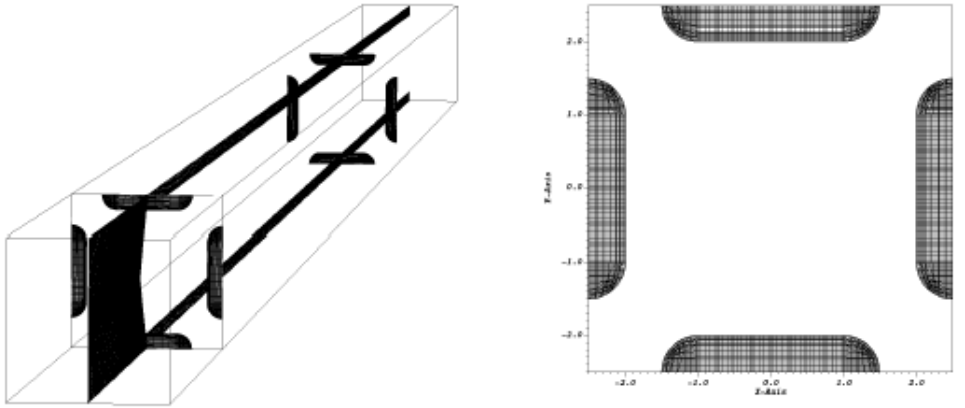
(b) O2

[1] J. Guo, N. A. Shaheen, and N. Hoyt, "Electrochemical Characterization of Molten Salt Chemistry During Atmospheric Ingressions," ANL/CFCT-23/30, Argonne National Laboratory (ANL), Argonne, IL (United States) (2023)

Mass Transfer to MSRE Subchannel

- MOSCATO has previously been used to calculate mass transfer correlations for various nuclear engineering geometries
  - Tube, tube bank, subchannel, pebble bed, etc. (see past MOSCATO reports).
- Recently, mass transfer to the reactor core was considered
  - Transport to the salt/core interface affects carbide formation and permeation of material into graphite matrix
- Objective:
  - Create a suitable core subchannel mass flow correlation that can be used by lower-order modeling tools

MSRE core (left and center) and graphite block arrangement (right) [1]



MSRE subchannel mesh in MOSCATO [2]

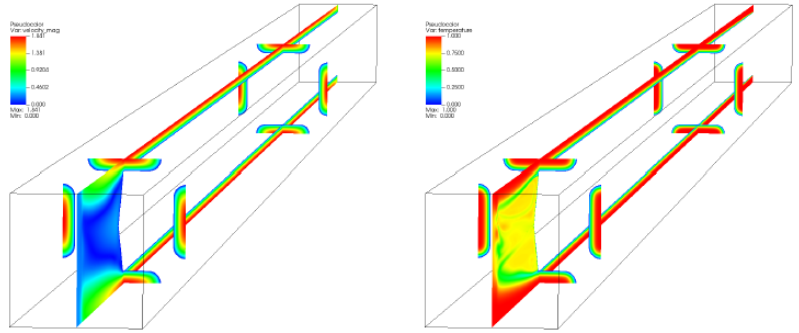
[1] H. MacPherson, “The molten salt reactor adventure,” Nuclear Science and engineering, 90 (4), pp. 374–380 (1985)
[2] A. Chaube, Large-eddy simulations of recirculation zones in channel-type molten salt reactors, PhD thesis, University of Illinois at Urbana-Champaign, 2021

Mass Transfer to MSRE Subchannel

- MSRE subchannel is an oval-shape cross section subchannel
  - High fidelity mesh is needed to capture high-Re behavior and narrow concentration boundary layers
- Improved correlations for transport to the MSRE core have been developed and provided to other partners within the NEAMS development community

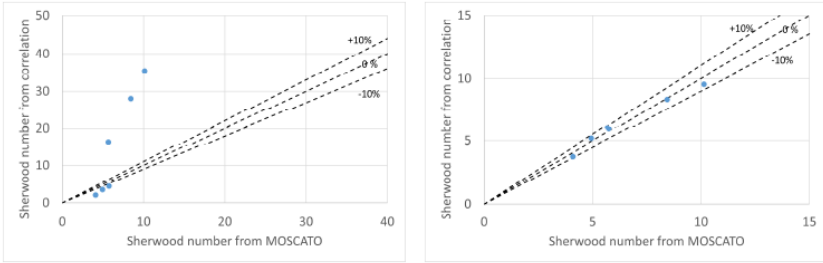
Sh / Sc \ $Re(Re_h)$	100 (156)	1000 (1560)
10	4.092	5.678
50	4.941	8.439
100	5.745	10.133

Sherwood numbers for MSRE core at different Re and Sc



(a) Velocity magnitude (b) Concentration

MSRE subchannel velocity and concentration profiles simulated by MOSCATO



(a) with original correlation (b) with adjusted correlation

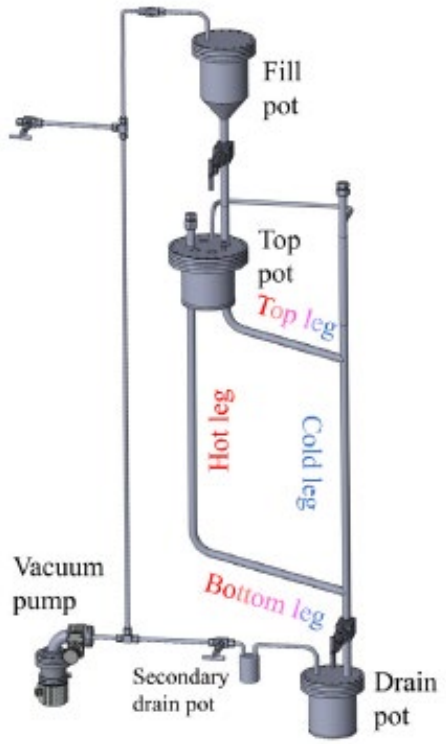
$$Sh = 0.0102 Re_h^{0.9} Sc^{1/3}$$

$$Sh = 0.844768 Re_h^{0.20706} Sc^{0.19632}$$

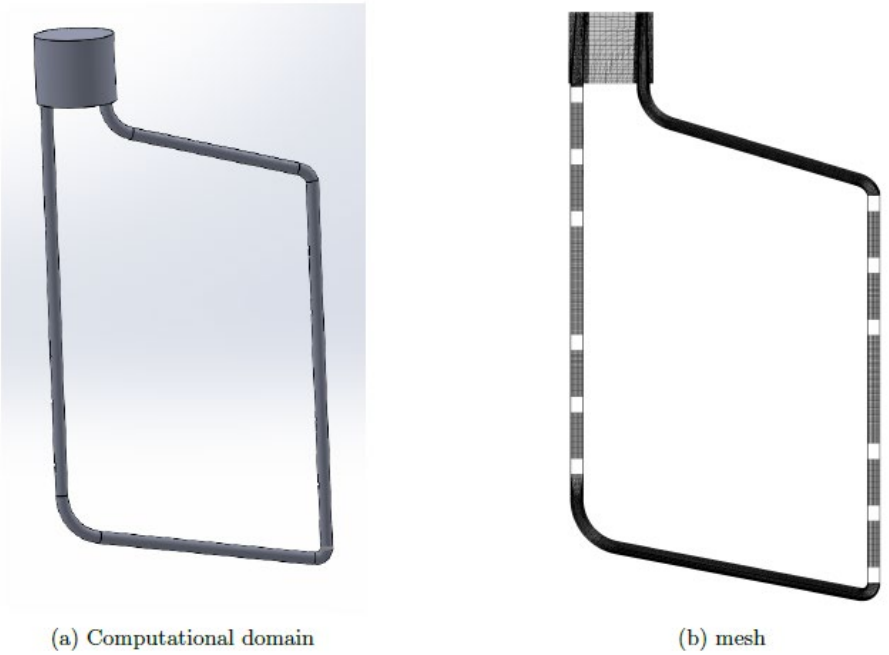
Traditional correlation and version modified for typical range of salt properties

Molten Salt Corrosion Validation

- Recent validation of corrosion modeling in MOSCATO demonstrated the solver's robustness
  - Flowing salt corrosion experiment (Raiman, et al.[1])
  - Thermally driven natural convection loop
  - Fully resolved alloy coupons are simulated in the middle of the pipe.
  - Salt: FLiNaK
  - System temperature: 600 C
  - Element diffusion coefficients from reference [2][3][4]
- **Physically-justified equations**
- **No need for tens of fit constants**
  - *Just one accounting for the unknown initial concentration of H+*
- **Direct validation to experimental data**



Experiment facility [1]



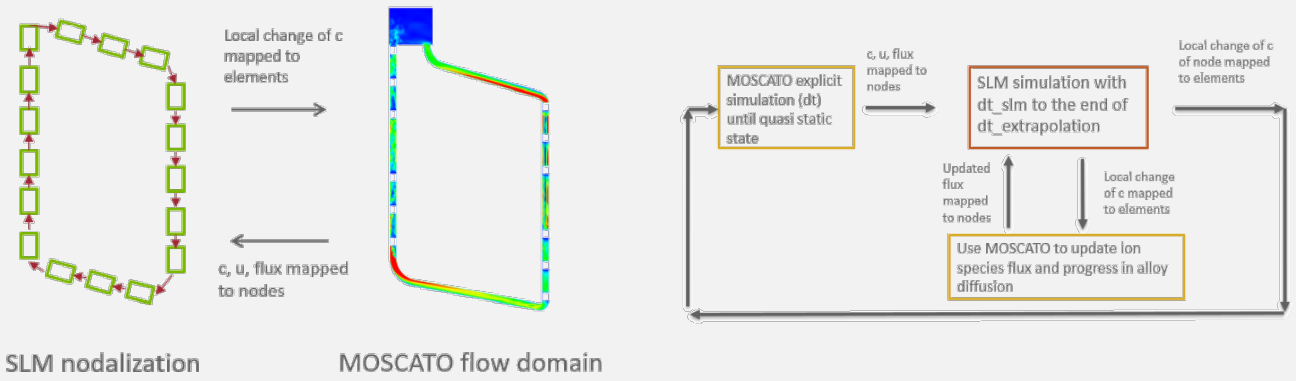
Computational domain and mesh in MOSCATO simulation

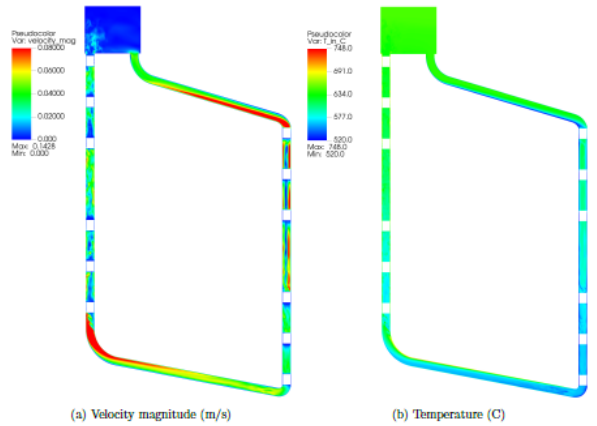
[1] S. S. Raiman et al., "Corrosion of 316H stainless steel in flowing FLiNaK salt," Journal of Nuclear Materials, 561, pp. 153551 (2022)
[2] S. B. Ping, F. et al., "Diffusion kinetics of chromium in a novel Super304H stainless steel," High Temperature Materials and Processes, 36 (2), pp.175–181 (2017)
[3] R. Patil and B. Sharma, "Lattice and grain-boundary diffusion of 59Fe in 316 stainless steel, "Metal Science, 16 (8), pp. 389–392 (1982)
[4] S. Bukovsk, et al., "Kinetics of nickel diffusion into austenitic stainless steels AISI 304 and 316L and calculation of diffusion coefficients," Materials, 16 (20), pp. 6783(2023)

Molten Salt Corrosion Validation

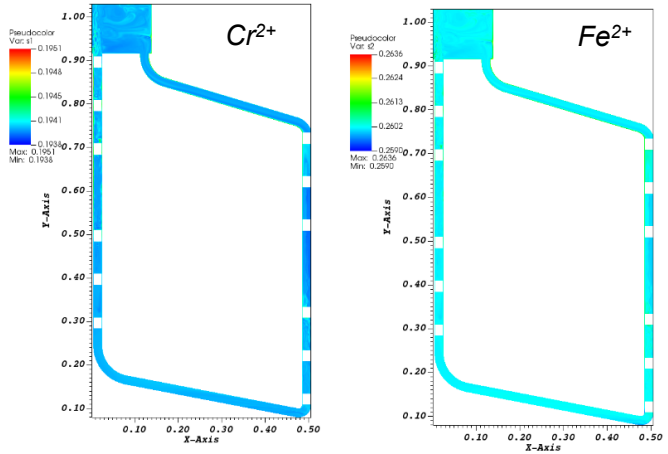
- MOSCATO Simulation Details:
  - The computational domain is fully meshed with samples inside the flow domain.
  - Salt species:
    - Cr^{2+}, Fe^{2+}, Ni^{2+}
    - H^{+} is also considered due to moisture in the original salt, but its initial concentration is unknown.
  - Extrapolation was done with the help of system level method
    - Nodalization of the system with data mapped back and forth to MOSCATO mesh enables longer time scales with larger time steps

System Level Nodalization Scheme to Enable High-Fidelity Simulations of Large-Scale Equipment





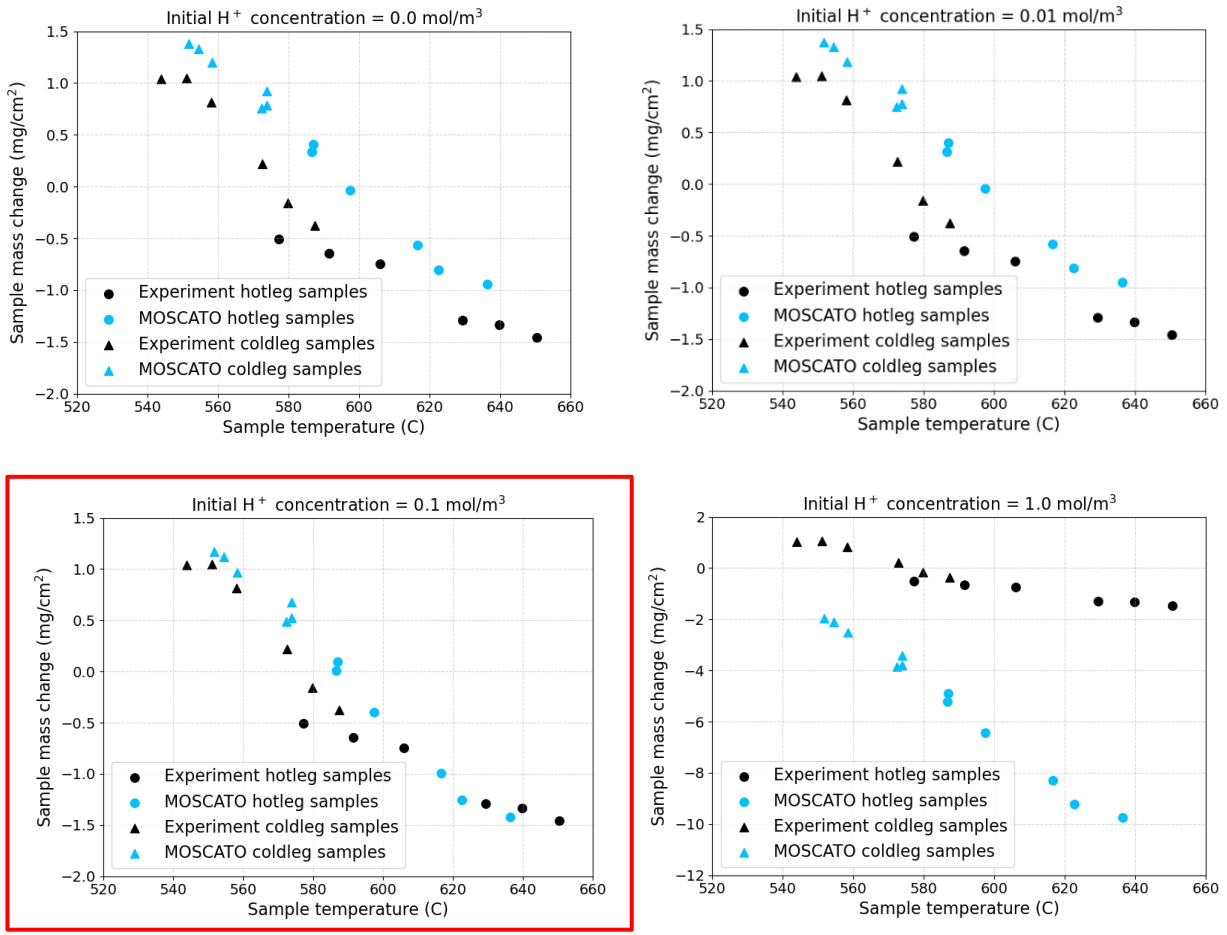
Velocity and temperature profiles



Cr^{2+} and Fe^{2+} concentration profiles

Molten Salt Corrosion Validation

- The initial H^+ concentration was not measured in the experiment even though this impurity affects the corrosion results significantly.
- A parametric study on H^+ concentration was performed using MOSCATO.
  - H^+= 0.0, 0.01, 0.1, 1.0, and 10 mol/dm^3
- Low initial H^+ impurities led to balanced losses and gains of mass on the hot and cold sides
- High initial H^+ impurities led to large losses of mass for both the hot and cold coupons
- A modest initial H^+ concentration (0.01 mol/dm^3) best matched the experimental results by showing a slight bias for higher mass losses on the hot side compared to the mass gains on the cold side



Coupon mass change after 1000 hr with different initial H^+ concentrations

Summary

- Additional modeling capabilities have been added to MOSCATO 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

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NEAMS MSR Chemistry/Corrosion Toolset