Development of Fission Gas and Species Transport Capabilities in SAM

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Molten Salt Reactor Program Annual Review

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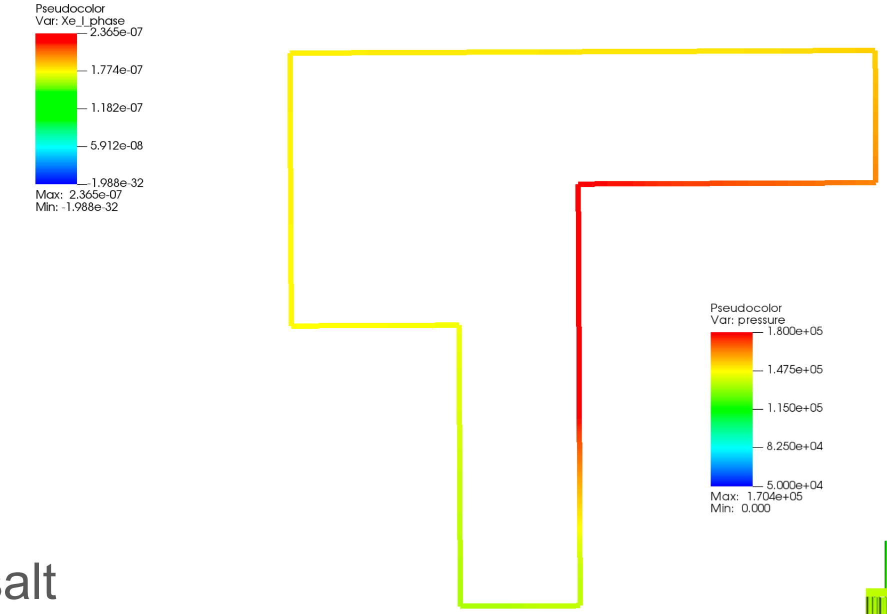
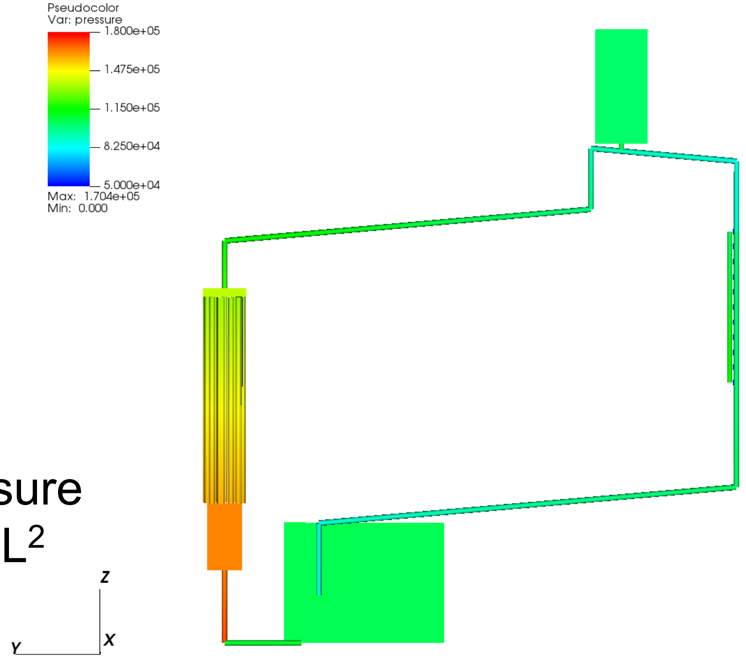
Introduction

- A modern system analysis code for advanced non-LWR safety analysis
  - Covers almost all non-LWR concepts
- Ongoing efforts to develop SAM for MSR applications
  - Salt thermophysical properties
  - Salt freezing
  - Species tracking for delayed neutron precursors and fission products in both salt and sparge gas
  - Species decay and decay heat
  - Species phase transfer
  - Modeling of non-condensable gas transport
- Validation using MSRE, MSR Campaign data, and open two-phase data



Prediction of salt xe-135 distribution in MSRE[1]

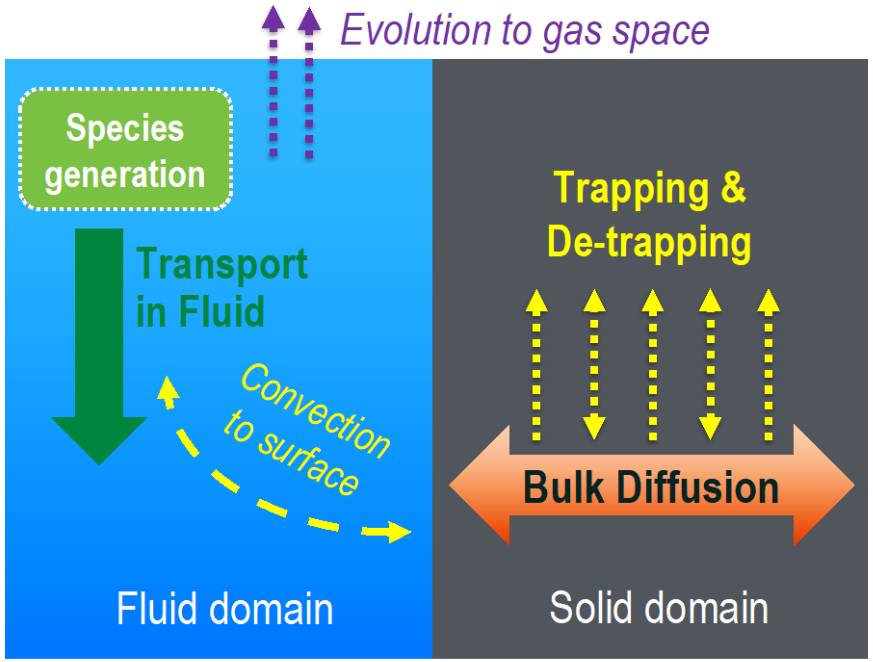


Prediction of pressure distribution in LSTL[2]

1. T. Mui, et al. "SAM Code Improvements for Molten Salt Reactor Transient and Species Transport Modeling", ANL/NSE-24/73, 2024.
2. Yoder, G., et al. "Development of a forced-convection liquid-fluoride-salt test loop", Proceedings of HTR, 2010

Species Tracking in SAM

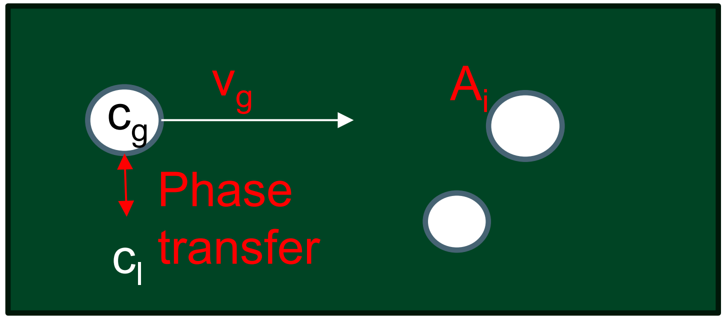
- Generic species (passive scalar) transport originally implemented in SAM to model flowing delayed neutron precursors in MSRs
- Framework expanded to simulate transport pathways of tritium in FHRs and MSRs
  - Collaboration with T. Fuerst on MSTTE modeling
- Ongoing work to consider additional applications:
  - Oxidation-corrosion in lead-cooled reactors
  - Redox corrosion in salt-cooled reactors
  - Noble gas/metal transport in MSR



Species transport pathways modeled in SAM

Enhancements to Species Tracking

- Species can now exist in the gas phase
  - Transported by gas velocity
- Phase transfer using Henry's Law for high-volatile gas
  - Henry and mass transfer coefficient calculated by Mole
  - Interfacial area and gas velocity by SAM
- Capture decay between species



Iodine transport in liquid

$$\frac{\partial I_l}{\partial t} + \frac{\partial (v_l I_l)}{\partial x} = -\lambda_I I_l + \gamma_I \bar{\Sigma}_f \Phi_f$$

Track decay from one species to another

Xenon transport in liquid

$$\frac{\partial Xe_l}{\partial t} + \frac{\partial (v_l Xe_l)}{\partial x} = -\lambda_{Xe} Xe_l + \lambda_l I_l - K_l A_i (Xe_g HRT - Xe_l)$$

Mass transfer data from Mole

Added phase transfer term

Xenon transport in gas

$$\frac{\partial Xe_g}{\partial t} + \frac{\partial (v_g Xe_g)}{\partial x} = -\lambda_{Xe} Xe_g + K_l A_i (Xe_g HRT - Xe_l)$$

Gas/bubble behavior predicted by SAM

Species can exist in gas phase

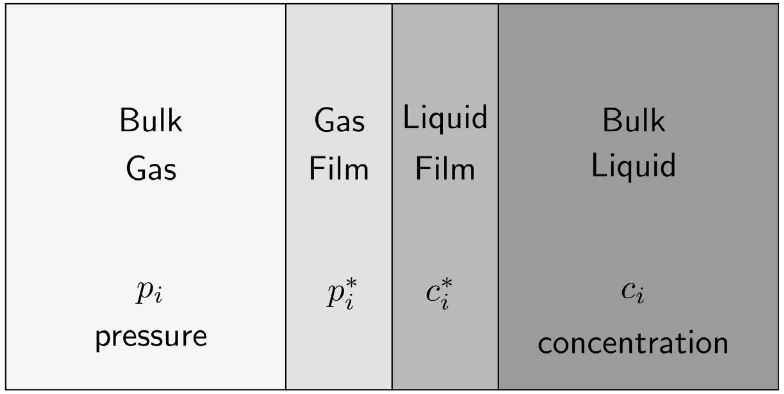
c: Species concentration (mol/m^3)
v: Species velocity (m/s)
λ: Species decay coefficient (1/s)
l/g: Liquid/gas phase index

I: Iodine concentration (#/m^3)
Xe: Xenon concentration (#/m^3)
A_i: Interfacial area (m^2/m^3)

K_l: Mass transfer coefficient (m/s)
H: Henry's coefficient (mol/m^3/atm)
R: Universal gas constant (J/mol/K)
T: Temperature (K)

Coupling to Saline and Mole

- Mole provides modeling of high-volatile species phase transfer[1]
  - Utilizes two-film theory
  - Provides Henry coefficients for FLiNaK and FLiBe salts and several noble gases
  - Mass transfer coefficient determined using Wilke-Chang or Stokes-Einstein[1]
- Saline is a C++/Fortran/Python interface to MSTDB-TP
  - Integrated into MOOSE and SAM
  - Provides thermophysical properties of many common salts and salt compositions



$$c_i^* = p_i H$$

$$p_i^* = c_i / H$$

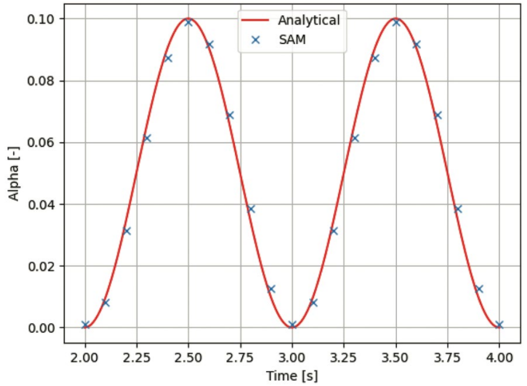
Gas liquid interface modeled using two-film theory

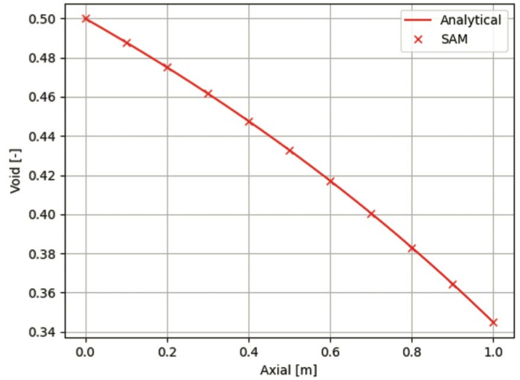
$$\Phi_j = K_j^L\left(p_j^g H_j - c_j^l\right) = K_j^G\left(p_j^g - c_j^l / H\right)$$

Interface concentrations determined using Henry's Law

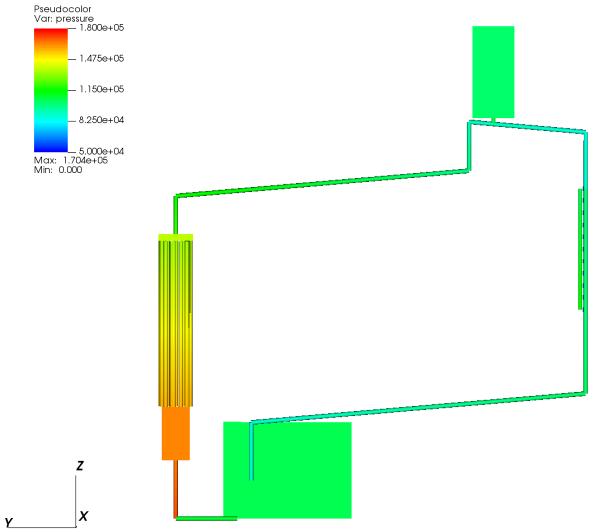
1. K. Lee, W. Williams, J. McFarlane, D. Kropaczek, and D. de Wet, "Semi-empirical model for Henry's Law Constant of Noble Gases in Molten Salts", Nature Portfolio, 14:12847, 2024, https://doi.org/10.1038/s41598-024-60006-9.

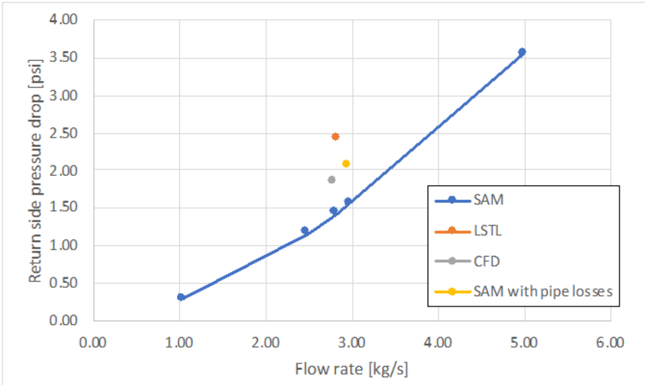
Verification and Validation Activities



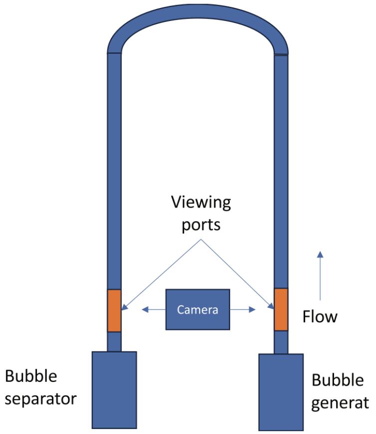


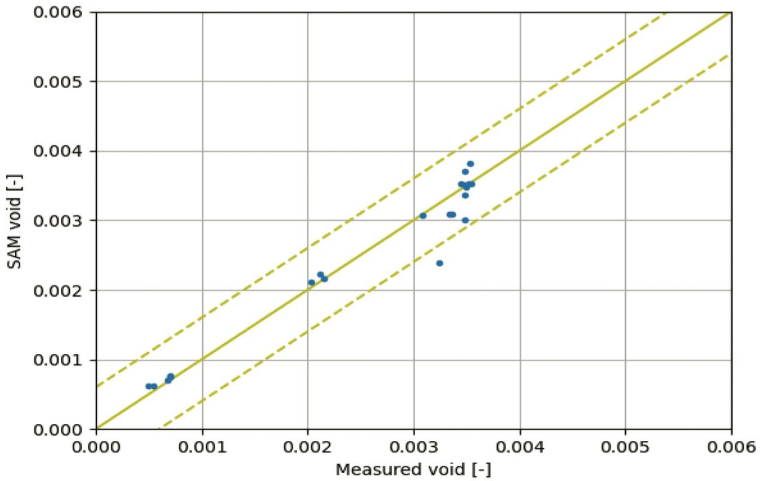
Development of verification test suite for gas transport model[3]



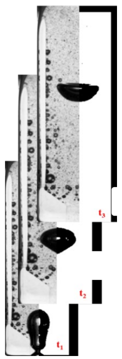


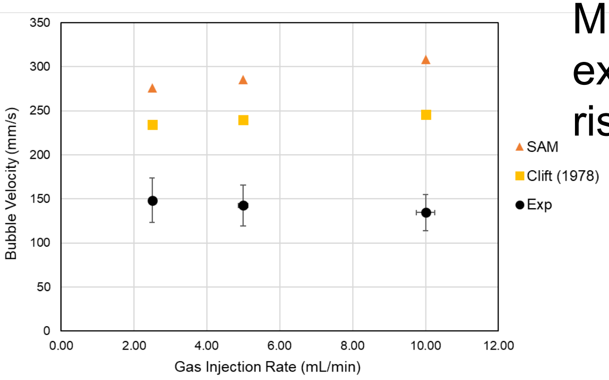
Modeling of pressure drop in LSTL[2]





Modeling of void fraction in Kress experiment[3]



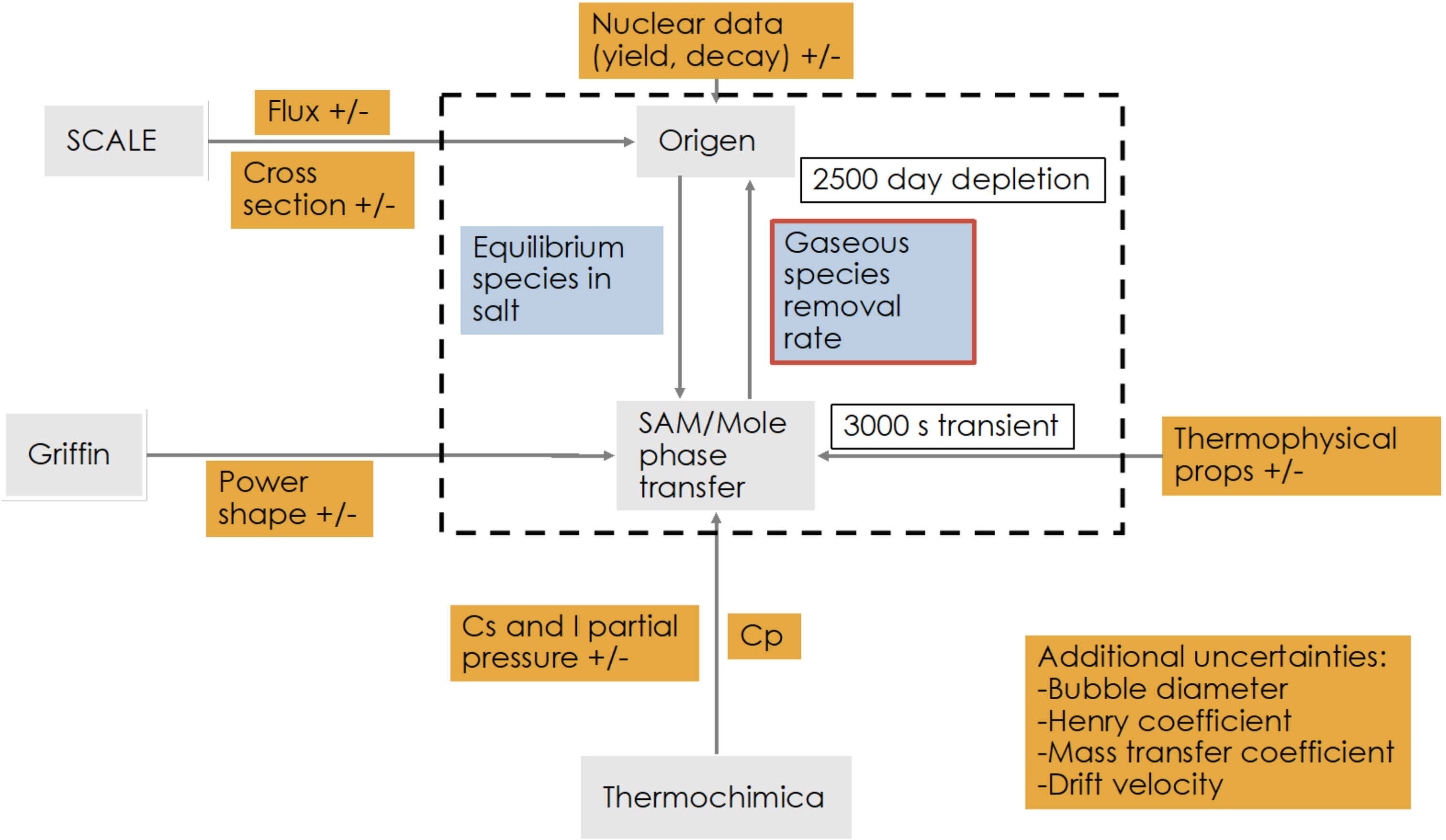


Modeling of experiments of bubbles rising in molten salt[1]

1. McFarlane, J., et al. “Design of Instrumentation for Noble Gas Transport in LSTL Needed for Model Development” Report. ORNL TM-2023-3138 (2023).
2. Yoder, G., et al. “Development of a forced-convection liquid-fluoride-salt test loop”, Proceedings of HTR, 2010
3. Salko, R, et al. “Implementation of a Drift Flux Model into SAM with Development of a Verification and Validation Test Suite for Modeling of Noncondensable Gas Mixtures”, Nuclear Technology, 2024

Modeling of Off-Gas System

- Model pool-type MSR
  - Bubble generation due to xenon creation and phase transfer
  - Species and bubble transport affects fission gas concentration in pool region
  - Bubble buoyancy leads to escape at pool surface
- Depletion determines fission product inventory

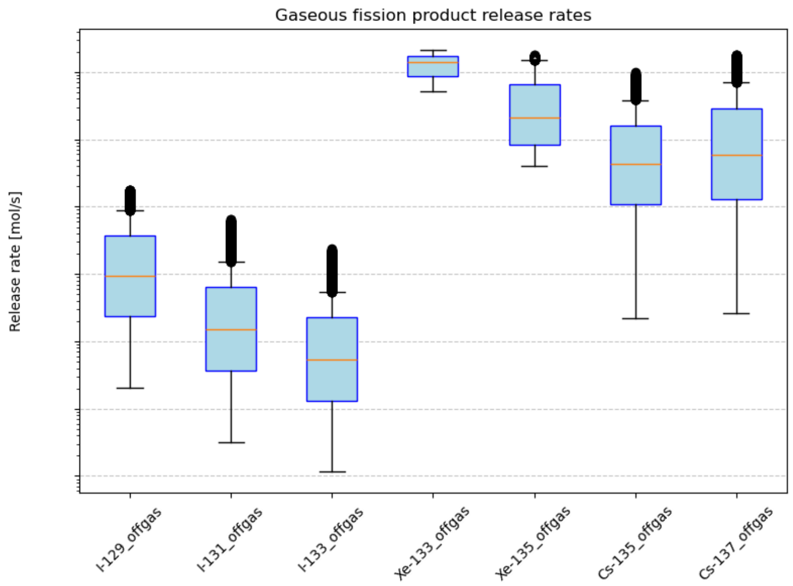


Coupled system being utilized for prediction of off-gas of fission products plus uncertainty[1]

1. DOE iFOA project in collaboration with Terrestrial Energy, USA

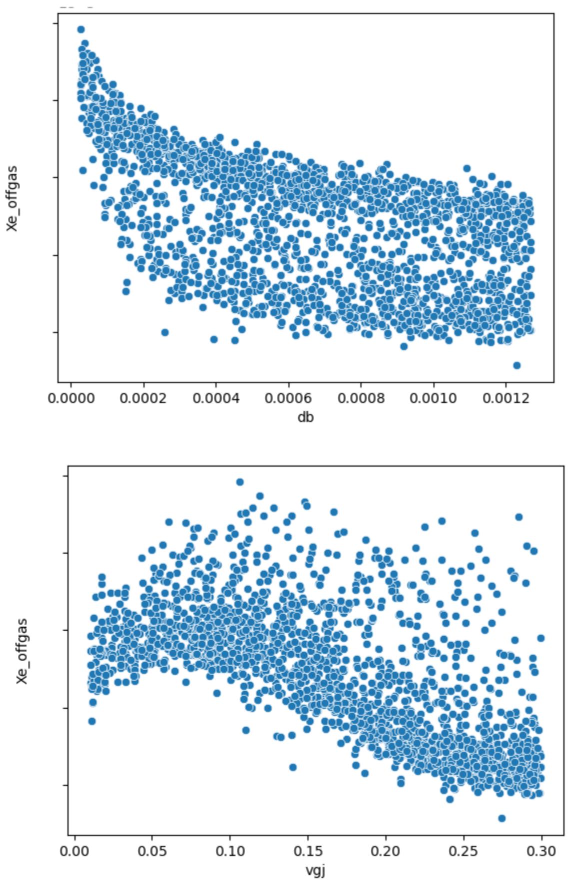
Uncertainty Quantification of Off-gas

- Forward UQ analysis of off-gas modeling
  - Variation of 15 input parameters
  - Nuclear data, thermophysical fluid properties, mass transfer data, bubble behavior
  - Xenon, cesium, and iodine off-gas rate are figures of merit (FOM)
  - 5,000 evaluations of coupled analysis lead to convergence of FOMs
- Bubble velocity uncertainty obtained from MSR Campaign data[1]



Spread in off-gas release rates due to input uncertainties

Bubble terminal velocity, bubble diameter, and thermochemical data found to be potentially high importance



Relationship between input parameters and off-gas rates

1. Daniel Orea, Kevin Robb, Joanna McFarlane, Comparative study between experimental measurements and model predictions of bubble rise velocity in molten LiCl-KCl, Nuclear Engineering and Design,Volume 443,2025,14247,ISSN 0029-5493,

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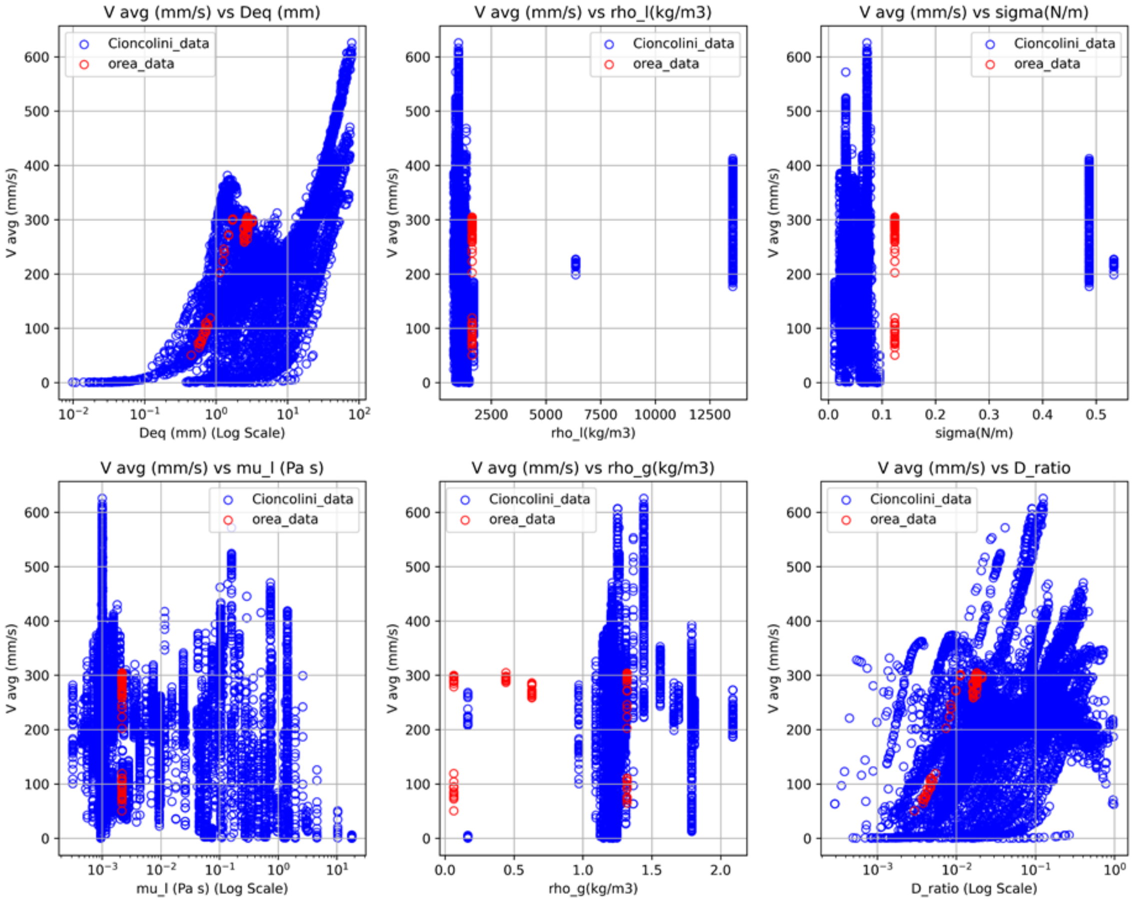
SAM Data Needs

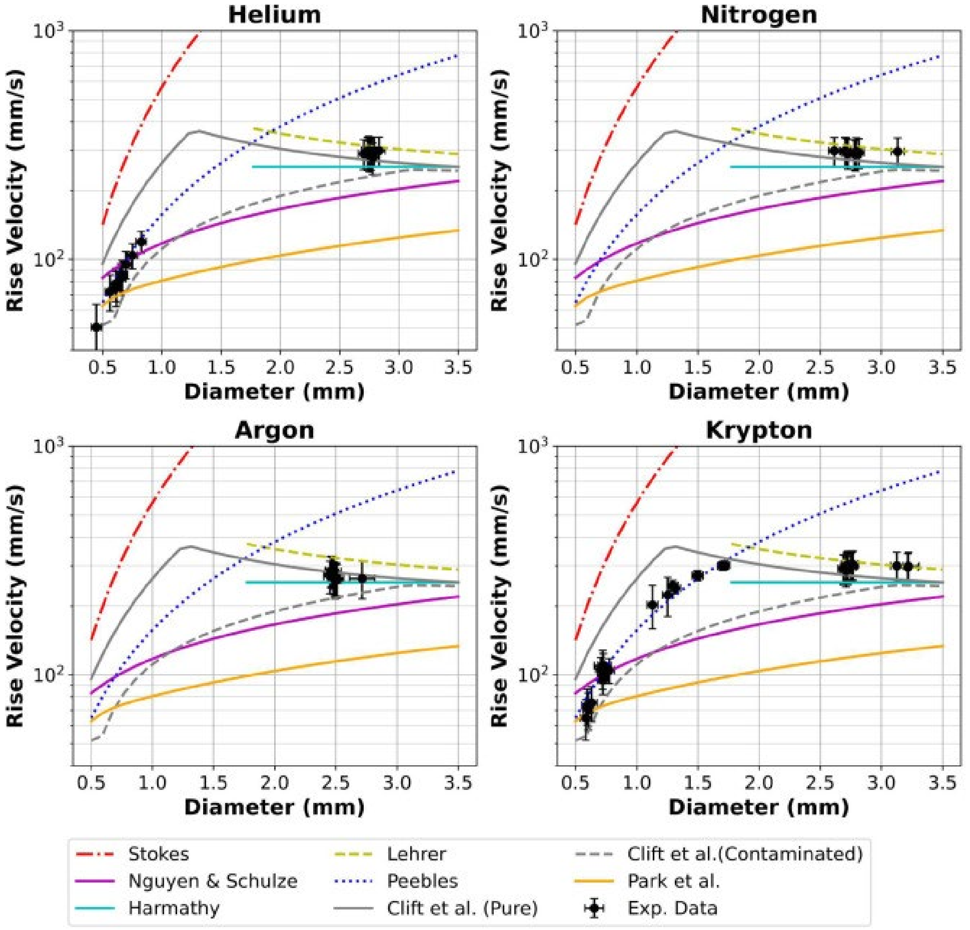
- Gas bubble behavior in stagnant and pumped salt systems
  - Bubble coalescence, breakup, interfacial effects on slip and buoyancy
- Mass transfer behavior due to phase change and solid interaction
  - Impact of noble metals
- Salt entrainment and transport at free surfaces



New salt data (red) produced by Orea[1] covers new two-phase conditions and is used for SAM development

1. Daniel Orea, Kevin Robb, Joanna McFarlane, Comparative study between experimental measurements and model predictions of bubble rise velocity in molten LiCl-KCl, Nuclear Engineering and Design,Volume 443,2025,14247,ISSN 0029-5493,

Modeling bubble rise in salt



Comparison of Orea data to selected models

$$\textbf{Harmathy:}\quad v = 1.53\left[\frac{\Delta\rho\, g\sigma}{\rho_l^2}\right]^{0.25} \quad \text{for } Re > 500$$

Original model implemented in SAM

$$\textbf{Clift:}\quad \begin{cases} v = 0.138 g^{0.82}\left(\frac{\rho}{\mu}\right)^{0.639} D_{eq}^{1.459} & \text{if } D_{eq} < 1.3\ mm \\ v = \sqrt{\frac{2.14\sigma_l}{\rho_l D_{eq}} + 0.505 g D_{eq}} & \text{if } D_{eq} \geq 1.3\ mm \end{cases}$$

Clift model recognizes bubble size

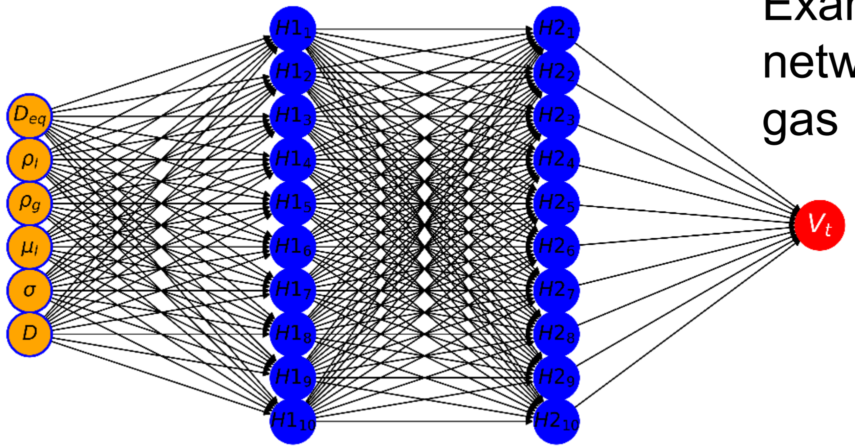
$$\textbf{DSM Clift}\quad \begin{cases} v = 0.136 g^{0.799}\left(\frac{\rho}{\mu}\right)^{617} D_{eq}^{1.459} & \text{if } D_{eq} < 1.75\ mm \\ v = \sqrt{\frac{2.366\sigma_l}{\rho_l D_{eq}} + 0.566 g D_{eq}} & \text{if } D_{eq} \geq 1.75\ mm \end{cases}$$

Modified form developed by Orea[1]

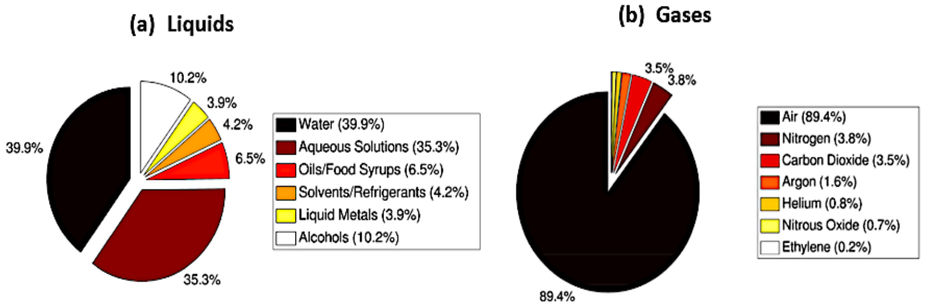
1. Daniel Orea, Kevin Robb, Joanna McFarlane, Comparative study between experimental measurements and model predictions of bubble rise velocity in molten LiCl-KCl, Nuclear Engineering and Design,Volume 443,2025,14247,ISSN 0029-5493,

Development of a new model using machine learning

- UTK led efforts to develop an ML model using three approaches:
  - Pure neural network trained on data
  - Physics informed neural network - use existing model to constrain neural network
  - Symbolic regression – discover model form
- Transfer learning techniques tested
  - Start with Cioncolini database[1] (7,000 data points)
  - Fine tune with Orea data
- Model implemented into SAM



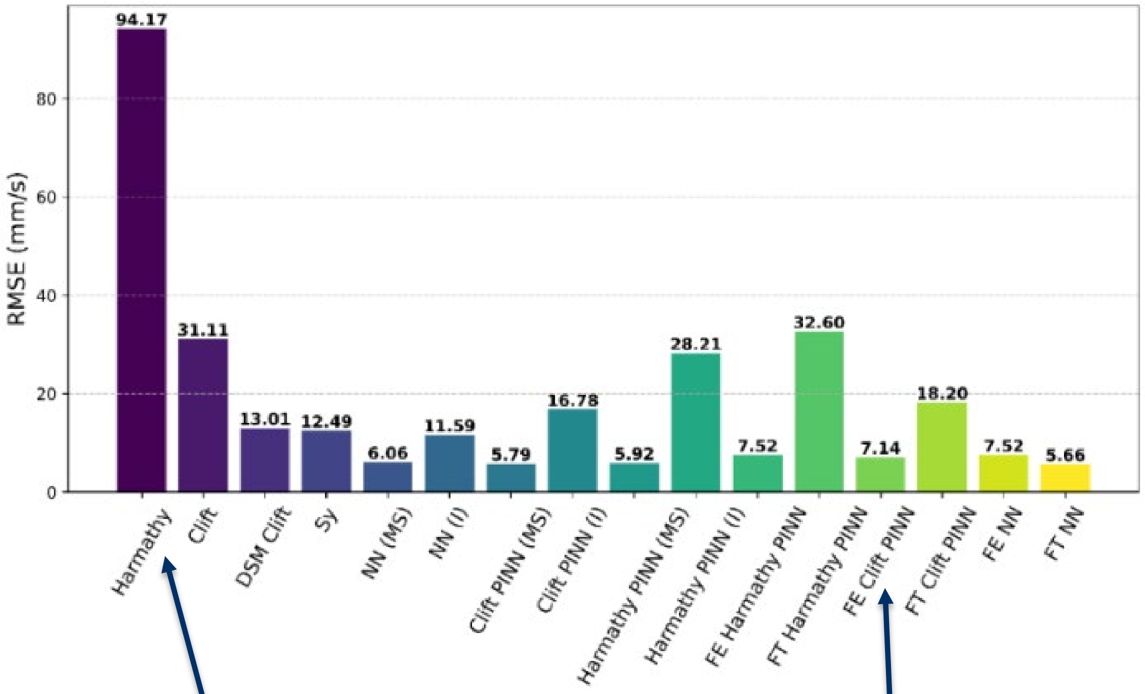
Example of neural network that predicts gas bubble velocity[2]



Large bubble database (non-salt) used to supplement model training using transfer learning

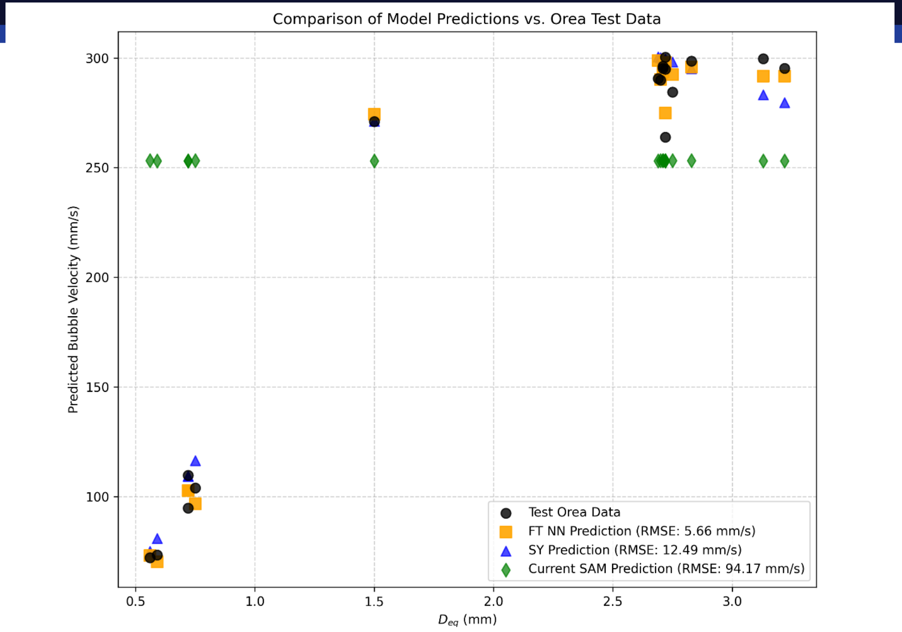
1. Cioncolini, A. and Magnini, M. (2025). Solitary bubbles rising in quiescent liquids: A critical assessment of experimental data and high-fidelity numerical simulations, and performance evaluation of selected prediction methods. *Phys. Fluids*, 37(2), 021304

Development of a new model using machine learning



Existing model performs poorly on Orea data

Both fine tuned NN and fine tuned PINN models perform best



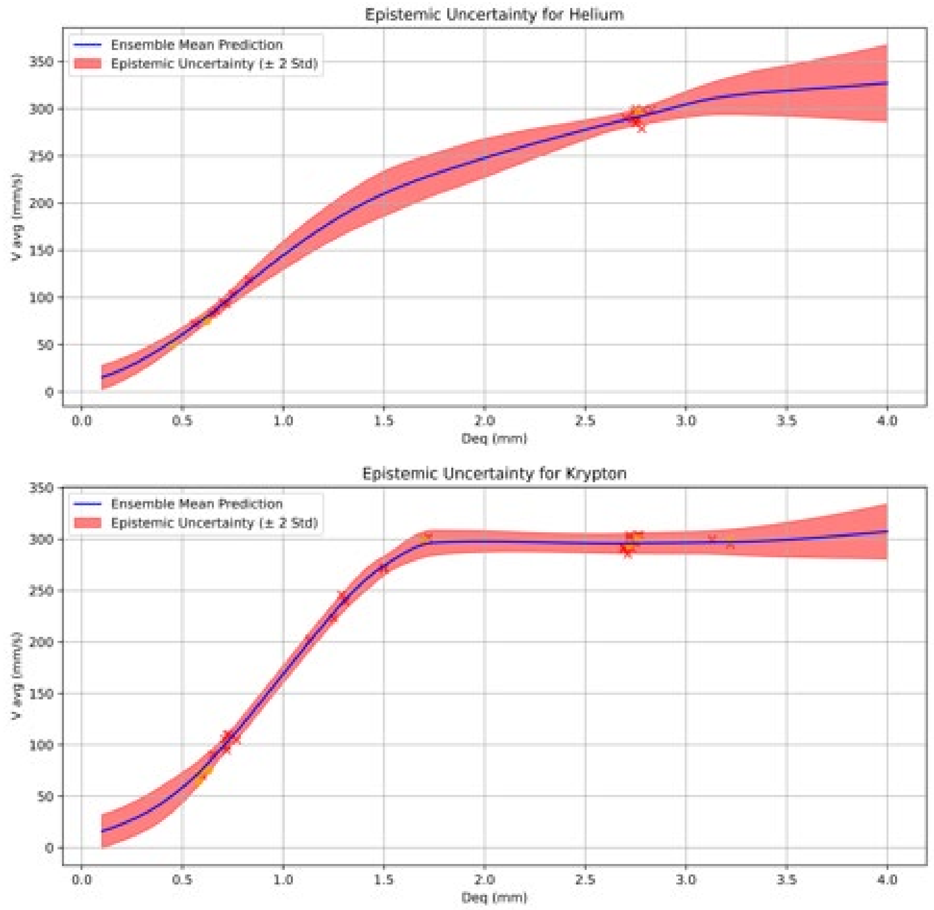
Comparison of models against Orea data

$$V_t = \frac{1.0065\,(D_{eq}\,g)^{0.5}}{exp\left(\frac{-1.9253}{Eo\,+\frac{0.11613}{E_O}}\right) + \left(\frac{37.741}{(Oh\,+\,0.44101)\,*\,Ar}\right) + 0.37981 + \,Oh}$$

Symbolic regression model

Including model uncertainty

- Deep ensemble used to quantify ML model uncertainty
  - Train many models with different initialization
  - Identifies epistemic and aleatoric sources of uncertainty
  - Regions of high uncertainty indicate future data needs for high impact model improvements



Model prediction and uncertainty for different bubble sizes can inform future data needs

Summary

- Species and gas transport modeling capabilities expanded in SAM for modeling of MSRs
  - Ability to track gaseous species using drift flux
  - Ability model phase transfer, decay between species, and bubble release
- Demonstration of capabilities shown by performing fission gas release uncertainty analysis
- Model is being expanded including coupling with Thermochimica, bubble modeling improvements based on MSR Campaign data, graphite xenon absorption, and improved coupling for depletion
- Future work on salt spill, improvements on noble gas and noble metal transport, and continued collaboration with MSTTE campaign
- Additional data in high uncertainty regions will improve model accuracy and uncertainty

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Enhancements to Species Tracking

- Mass transfer correlations developed from high-fidelity MOSCATO/NekRS[1] have been integrated into SAM
- Porous diffusion of species in solids also modeled (e.g. Xe in graphite)
  - Dissolved fluid species transfers to graphite pore space through a two-film model
  - Knudsen diffusion within pore gas space
- Species reactivity feedback added to PKE model to account for evolution of Xe-135 concentration
  - Reactivity feedback will integrate provided reactivity coefficients with species concentrations and volume over axial length for gas/liq/solid phase
  - Integrated into SAM Point Kinetics model, work is ongoing to demonstrate using MSRE

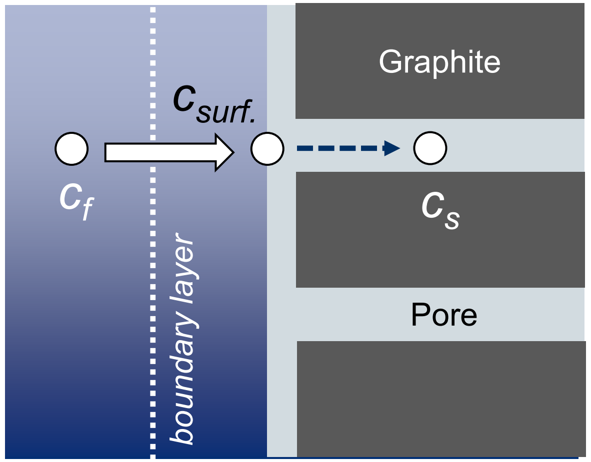
Species porous diffusion in solids (Xenon in graphite)

$$\frac{\partial c_s}{\partial t} - \frac{D_{Xe,s}}{\varepsilon}(\nabla^2 c_s) - \lambda_{Xe} c_s = 0$$

Fluid-solid interface species flux

$$J_{xe} = k_m\left(c_f - HRT\varepsilon^{-1} c_{s,surf.}\right)$$

c: Species concentration (#/m³)
λ: Species decay coefficient (1/s)
l/g: Liquid/solid phase index
D: Effective diffusivity (m²/s)
ε: Porosity
k_m: Mass transfer coefficient (m/s)



Species convection and diffusion in porous structures

Species reactivity feedback

$$\rho_{species} = \sum_{n}^{N} \alpha_n c_{phase}(t) V_{phase}$$

ρ: Reactivity (Δk/k)
α: Species reactivity coefficient (Δk/k per #)
c: Species concentration (#/m³)
V: Volume of phase (m³)

1. H. Yuan and N. Hoyt, "MOSCATO Development and Integration in Fiscal Year 2023", ANL/NSE-23/50.