Noble metal transport in an MSR heat exchanger with NekRS/MOSCATO

Haomin (Kirk) Yuan, Jun Fang, Tingzhou Fei

Nuclear Science and Engineering Division, Argonne National Laboratory

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Outline

- MSR heat exchanger
  - Motivations
  - Simulation setups
  - Preliminary results
- Noble metal deposition model development
  - Model implementation in MOSCATO/NekRS
- Summary

Noble Metal Deposition

- During operation of molten salt reactors (MSRs), noble metal fission products such as ^{125}Sb, ^{106}Re, etc. are generated in the fuel salt and may deposit on:
  - Structure surfaces such as heat exchanger
  - Graphite surfaces and subsequently penetrate the graphite pore structure.
- Post-irradiation examination of the Molten-Salt Reactor Experiment (MSRE) demonstrated significant accumulation of noble metal activity in graphite stringer samples and on structural surfaces.

Motivation

- **Prevent Heat Exchanger Fouling:** High-fidelity CFD predicts the significant plate-out of noble metals—which accounted for 40% of all deposition in MSRE U-235 runs—to prevent tube clogging and degraded heat transfer
- **Account for Localized Decay Heat:** Multiphysics modeling captures the intense, localized decay heat generated by accumulated radioactive particulates, which is necessary to prevent unpredicted structural damage or thermal-hydraulic shifts
- **Define the Radioactive Source Term:** Tracking fission product migration and transmutation accurately defines the fuel composition and the reactor's source term, which is crucial for material accountancy and designing effective radiation shielding

Simulation Setup: Geometry

- Targeting high-fidelity realistic geometry of MSRE PHX

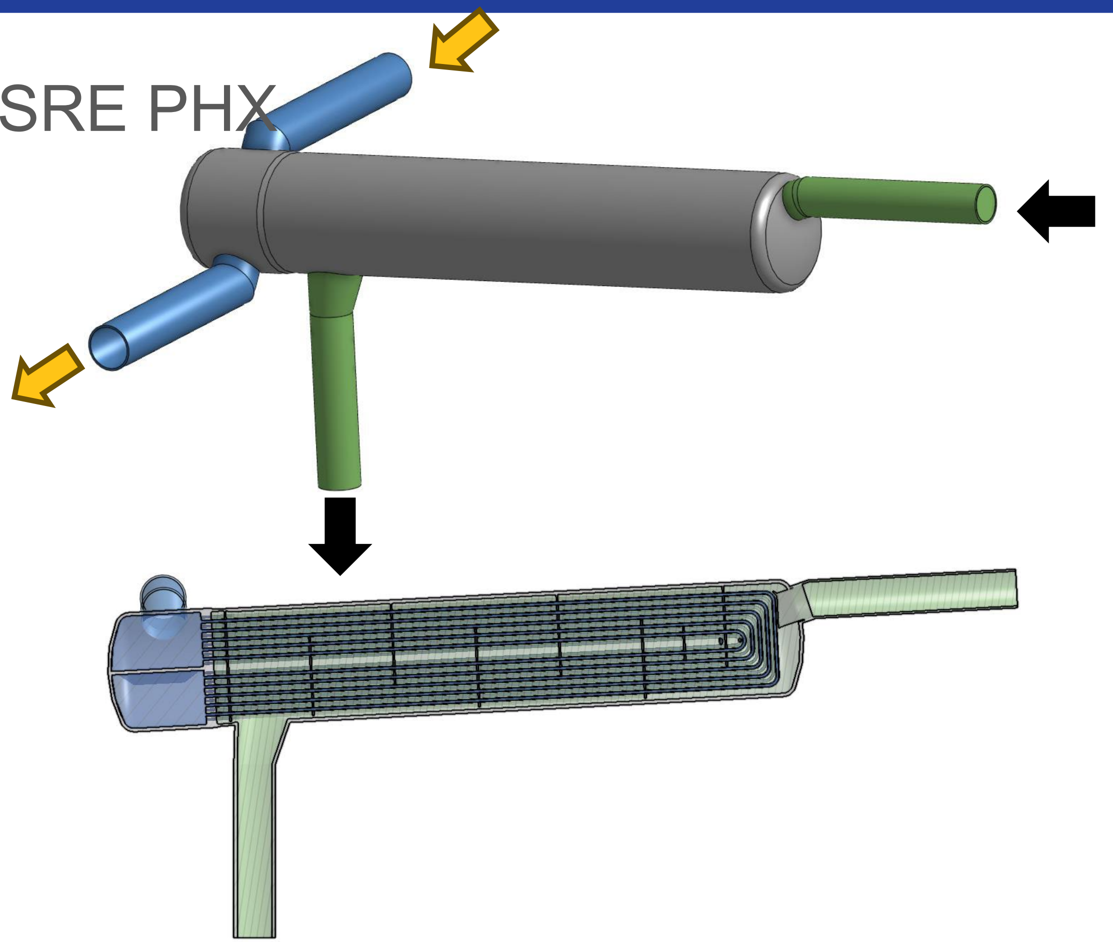
PHX Shell-Side Geometry Highlights

Overall Dimensions: Approximately **2.5 m long** and **0.43 m** in outer diameter.

Tube Bundle: Contains **159 U-shaped tubes** (12.7 mm outer diameter) arranged in an equilateral triangular pitch.

Internal Baffling: Features cross-baffles with a 25% cutaway to force crossflow (12 *in* apart), an impingement baffle to disperse inlet flow, and a solid barrier plate to protect the tube sheet.

Nozzles: Uses a 5-inch angled inlet and a slanted conical reducer at the outlet (narrowing from 17.8 cm to 12.7 cm) to minimize pressure drop



The CAD model of the MSRE PHX is shown, with green pipes indicating the inlet and outlet of the shell-side flow passage (*Credit: Akner, 2021*).

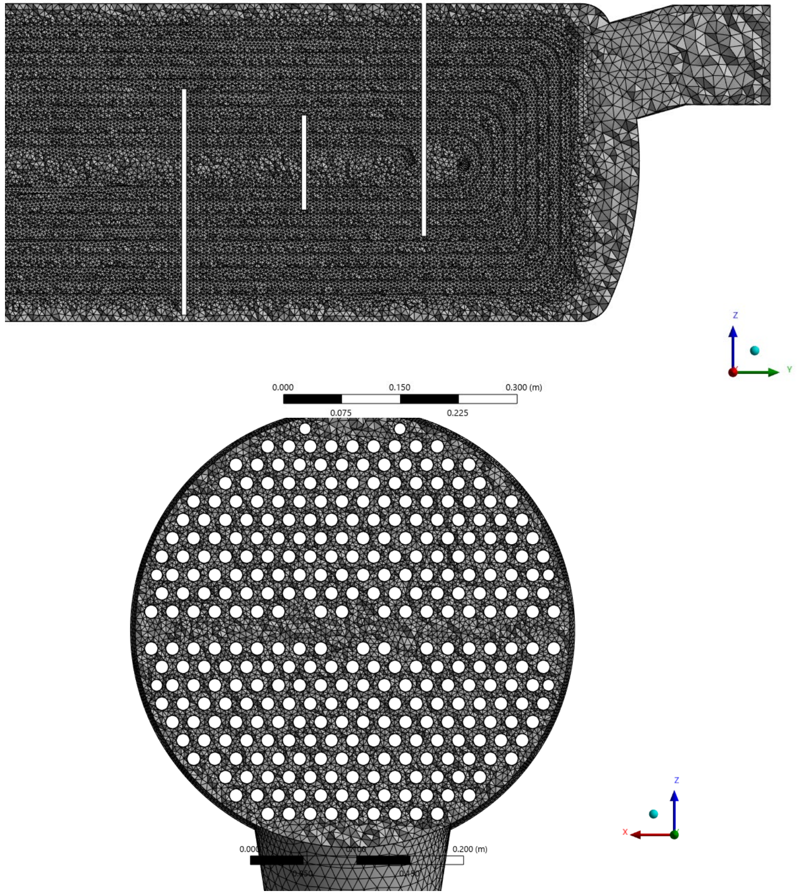
Simulation Setup: mesh generation

- Balancing mesh quality with overall computational mesh size

Creating a high-quality CFD mesh is non-trivial. Multiple iterations were required to produce a mesh suitable for the solver, while minimizing stability issues related to poor mesh quality and highly stretched cells.

An initial tetrahedral mesh was generated using ANSYS Mesh and subsequently converted into a hexahedral mesh using an in-house **tet-to-hex utility** (*Yuan et al., 2020*). The final mesh consists of approximately **56 million hexahedral cells.**

Refined boundary layer mesh was applied to accurately capture steep velocity and temperature gradients near the wall surfaces.



Hybrid tet-wedge mesh generated in ANSYS

Simulation Setup: Representative flow Conditions

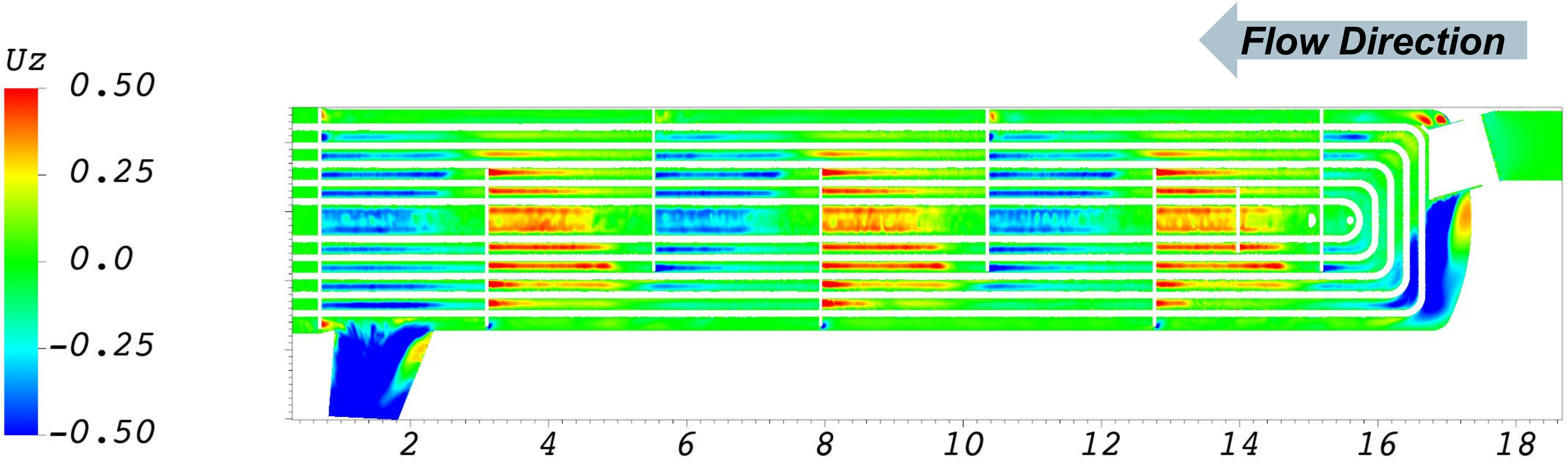
A molten salt composition of **$LiF–BeF_2–ThF_4–ZrF_4–UF_4$** (*ORNL-TM-2098*) is used.

At the design flow rate of 1,200 gpm, the Reynolds number at **the PHX inlet** is approximately **248,000**, while the local Reynolds number within **the tube bundle** is around **7,000**.

Given the strongly turbulent flow conditions, an **unsteady RANS** (URANS) approach is employed to model the turbulence using **nekRS**.

Parameter	Value	Unit
Fuel Salt Composition	$LiF - BeF_2 - ThF_4 - ZrF_4 - UF_4$	–
Density	2466	kg/m^3
Dynamic Viscosity	0.0075	$Pa \cdot s$
Kinematic Viscosity	3.04×10^{-6}	m^2/s
PHE Inlet Diameter	0.1275	m
PHE Inlet Fuel Velocity	5.93	m/s
Hydraulic Diameter of Tube Bundle	2.56×10^{-2}	m
Expected Fuel Velocity (Tube Bundle)	0.845	m/s
Local Reynolds Number (PHE Inlet)	248,486.21	–
Local Reynolds Number (Tube Bundle)	7,119.04	–

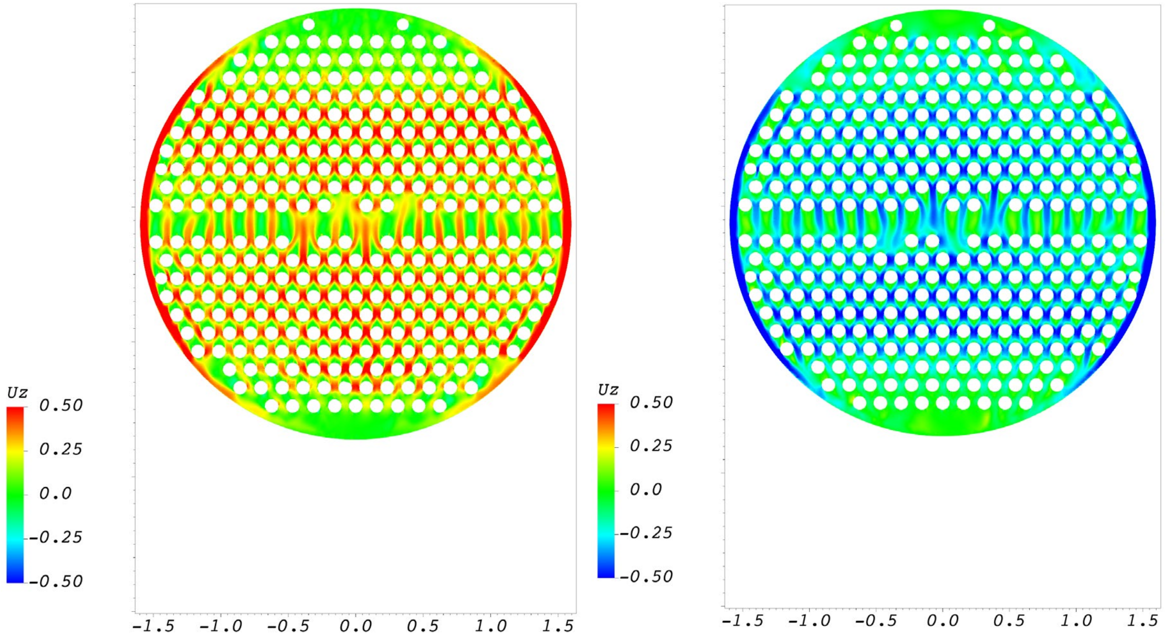
Converged Velocity Distribution



Vertical velocity field (U_Z) showing fuel salt entering at the right and flowing toward the outlet, with baffle plates inducing a characteristic zig-zag cross-flow. High-velocity regions occur at baffle window gaps, while low-velocity recirculation zones form behind the baffles.

Converged Velocity Distribution

- **Capturing Complex Flow:** *nekRS* CFD simulations successfully capture the stabilized, highly turbulent flow distribution inside the PHX shell, paving the way for high-fidelity temperature and fission product concentration mapping.
- **Predicting NM Plate-Out:** We are actively developing and validating a noble metal deposition model. This will be applied to our large-scale PHX simulations to accurately account for NM accumulation on the heat exchanger tubes and baffles.
- **MOSCATO Integration:** Combining the CFD model with *MOSCATO* will unlock full multi-physics capabilities, allowing us to study the feedback between NM deposition, localized decay heat, and potential heat transfer degradation in detail.



Vertical velocity field (U_Z) with zig-zag cross-flow

Noble Metal Deposition Model

- The noble metal deposition models on structure surface and graphite surface are different but share some similarity:
  - Unlike in structure, noble metal will diffuse into graphite interior.
- The transport and deposition of noble metal fission products (e.g., 106Ru and125Sb) in MSRE graphite are modeled using a one-dimensional diffusion–reaction framework.
- The model describes the migration of mobile species within graphite pores and their subsequent immobilization on internal graphite surfaces.
- The physical system considered is a graphite block exposed to circulating molten salt containing dissolved noble metal species.

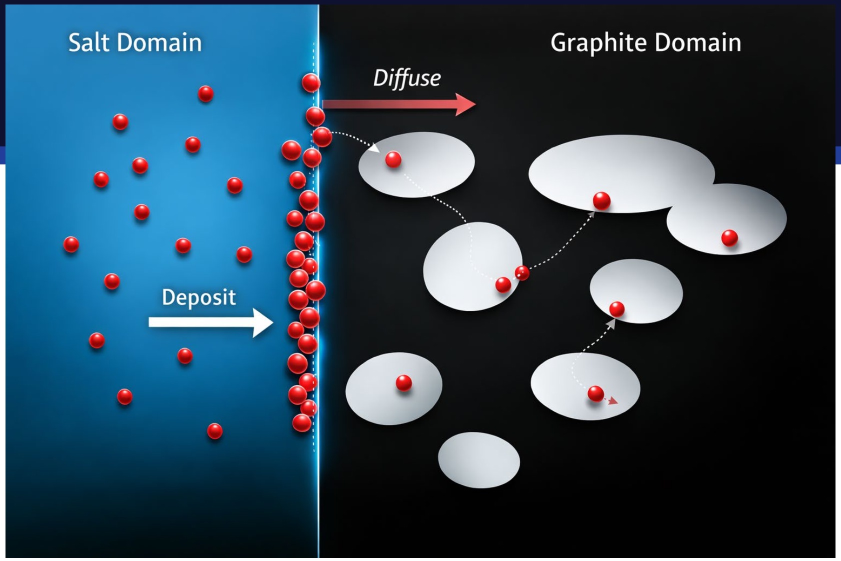


Diagram of noble metal particle deposit and migrate in graphite

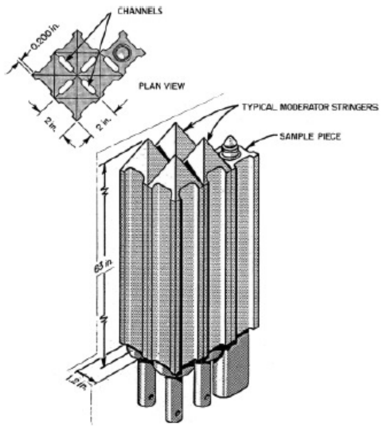


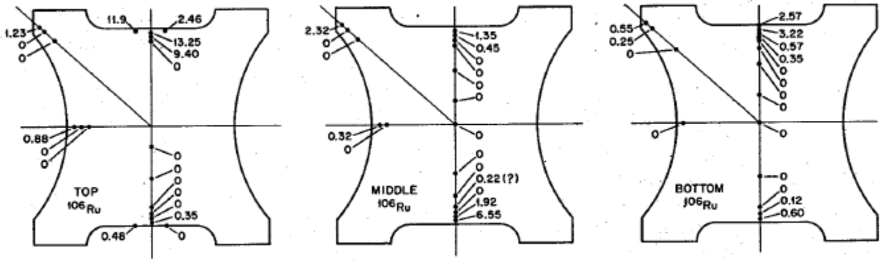
Figure 4.3: A diagram of the MSRE stringer (reproduced from [4]).

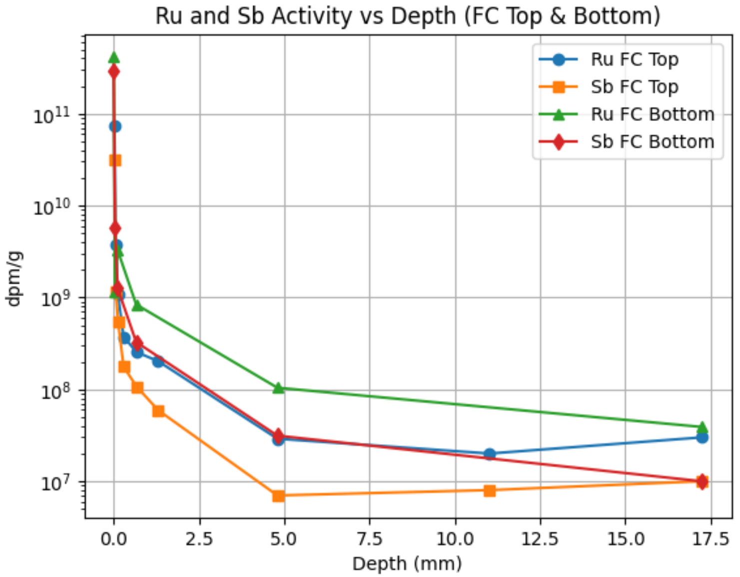
MSRE core graphite stringer [1]

1. A. Chaube, *Large-Eddy Simulations of Recirculation Zones in Channel-Type Molten Salt Reactors*, M.S. thesis, Dept. Nuclear, Plasma & Radiological Eng., Univ. of Illinois Urbana-Champaign, Urbana, IL, USA, 2021.

Noble Metal Deposition Model

- From MSRE report (ORNL-4728)
  - Graphite from MSRE core was examined (1971) after MSRE (1965-1969) was shutdown.
  - 4 years of cumulative exposure
    - But only 11515 hours (480 days) of effective operation time.
  - Activity was measured in the graphite
    - 106Ru, 125Sb, 134Cs, 137 Cs, etc
    - We focus on 106Ru for now





Measurement of noble metal activity on graphite surface and interior [1]

1. M. W. Rosenthal, R. B. Briggs, and P. N. Haubenreich, *Molten-Salt Reactor Program Semiannual Progress Report for Period Ending August 31, 1971*, Oak Ridge National Laboratory, Oak Ridge, TN, USA, Rep. ORNL-4728, Feb. 1972.

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Noble Metal Deposition Model

- Governing equations:
  - In graphite porous structure [1]:
    - $C_m(x,t)$: mobile species concentration in graphite (mol/m^3)
    - $C_f(x,t)$: fixed (immobilized) species concentration (mol/m^3)
    - For structure, this part can be neglected

$$\frac{\partial C_m}{\partial t} = D\frac{\partial^2 C_m}{\partial x^2} - k_f C_m - \lambda C_m$$

$$\frac{\partial C_f}{\partial t} = k_f C_m - \lambda C_f$$

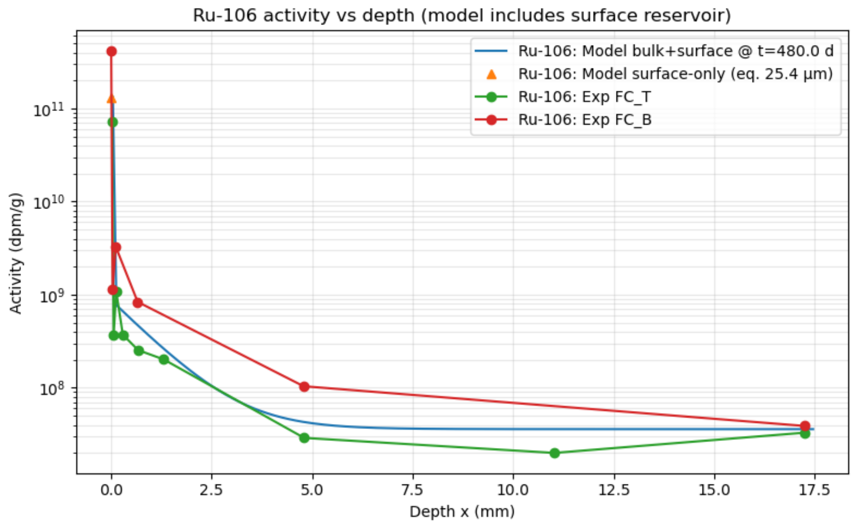
  - On graphite-salt interface [2]:
    - Surface Reservoir Model: this is need to model high activity on surface
    - S: surface species concentration (mol/m^2)
    - For structure, only need this part

$$\frac{dS}{dt} = f_s J_{in} - k_r S - \lambda S$$

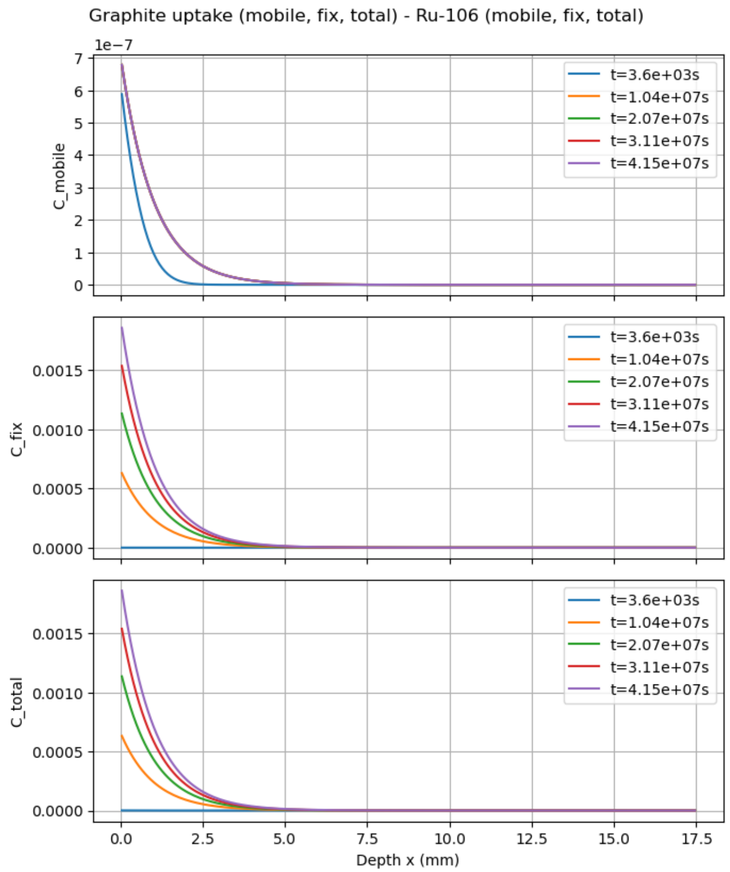
1. R. J. Kedl. A model for computing the migration of very short-lived noble gases into msre graphite. Technical Report ORNL-TM-1810, Oak Ridge National Laboratory, Oak Ridge, Tennessee, 1967.
2. H. Scott Fogler. Elements of Chemical Reaction Engineering. Prentice Hall, 4th edition, 2006.

Noble Metal Deposition Model

- One-dimensional model compared with experimental data
  - Mobile concentration (c_mobile) reached steady state very quickly.
  - Fixed concentration (c_fix) was accumulated in time.
  - The activity profile matched experimental measurement.
    - With uncertain parameters tuned



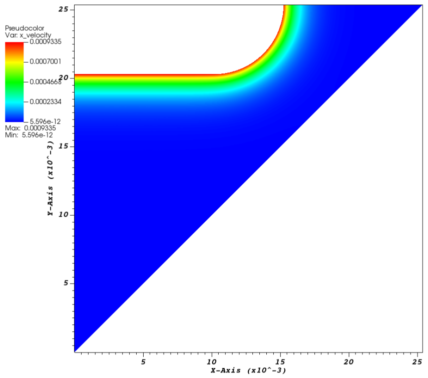
Activity profile from 1D model and compared with MSRE samples (480days)



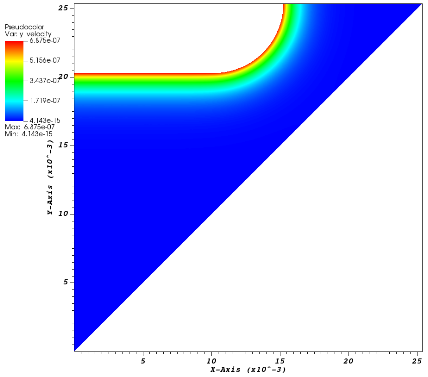
Concentration profile from 1D model

Noble Metal Deposition Model

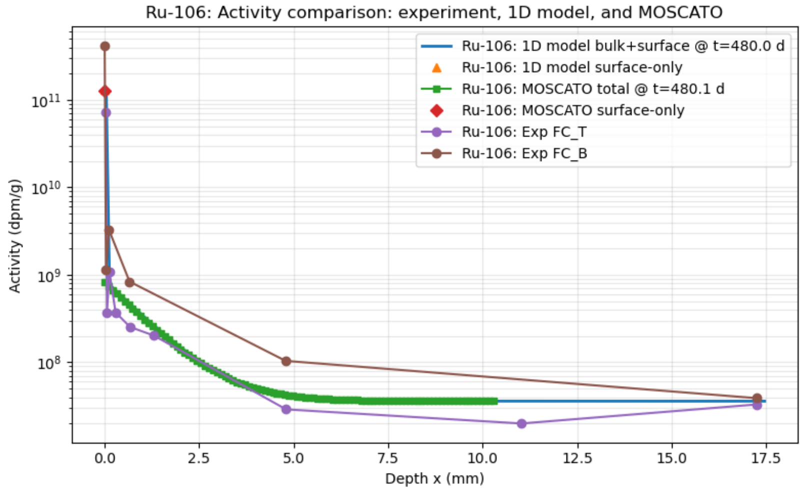
- The proposed model was also implemented in MOSCATO/NekRS
  - Currently only applied to a small section of the MSRE core graphite stringer
  - Will be applied to MSRE heat exchanger case later, with comparison with experimental measurement.



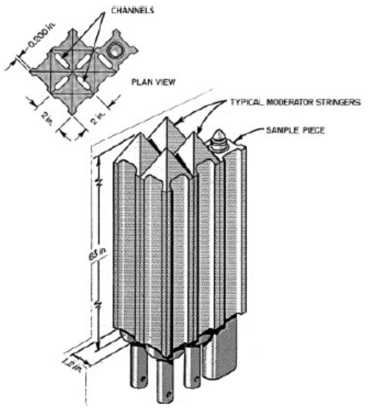
c_fix



c_mobile



MOSCATO result (480days)



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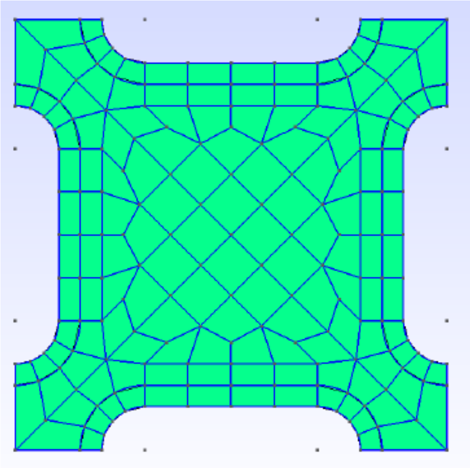

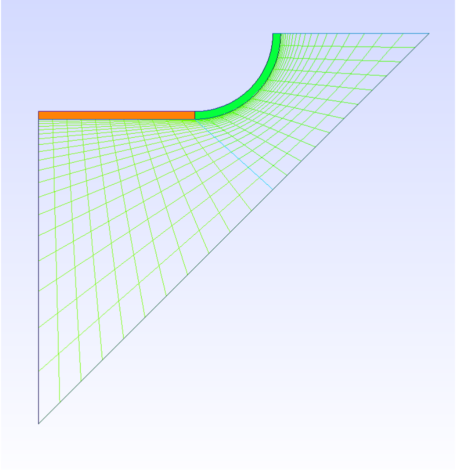

MSRE core graphite stringer

Subchannel graphite mesh

Summary

- High-fidelity CFD simulation was performed for MSRE heat exchanger using NekRS/MOSCATO
  - Velocity field was converged.
  - Ready for temperature and noble metal deposition simulation.
- Noble metal deposition model was developed and implemented NekRS/MOSCATO
  - Preliminary validation was performed for graphite using MSRE experimental measurement
  - The implemented model will be applied to MSRE heat exchanger in the future work

- Questions?
  - Please contact Haomin(Kirk) Yuan (hyuan@anl.gov) and Jun Fang (fangj@anl.gov)

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