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Molten Salt Reactor PROGRAM

Source Term Development for the MELCOR Severe Accident Code

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Sandia National Laboratories

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MELCOR for Advanced Nuclear Energy Technologies

Fully integrated, engineering-level code

- Thermal-hydraulic response of reactor coolant system, reactor cavity, rector enclosures, and auxiliary buildings
- Core heat-up, degradation and relocation
- Core-concrete interaction
- Flammable gas production, transport and combustion
- Fission product release and transport behavior

Level of physics modeling consistent with

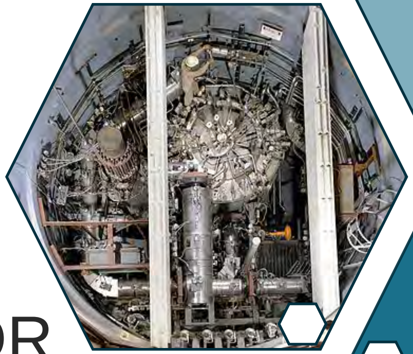
- State-of-knowledge
- Necessity to capture global plant response
- Reduced-order and correlation-based modeling

Traditional application

- Models constructed by user from basic components (control volumes, flow paths and heat structures)
- Demonstrated adaptability to range of reactor designs – LWR, LWR-SMR, FHR, HPR, HTGR, MSR, SFR, ATR, VVER, SFP…

Molten Salt Reactor Modeling

- Molten Salt Reactor mechanistic source term modeling strategies in MELCOR boil down to 3 primary concepts:
  1. Control
  2. Cool
  3. Contain
- MELCOR capabilities have been primarily tested using the MELCOR model of the MSRE
  - Liquid Salt Test Loop model (under development) will be added to the MELCOR validation matrix as data becomes available



Control

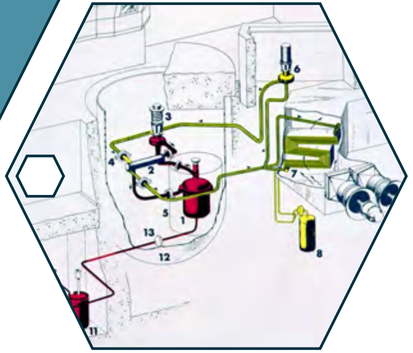
Fluid point kinetics, transmutatio
n

Cool

Generalized EOS, CVH, HS

Contain

Radionuclid
e species, transport, and retention



Images from https://en.wikipedia.org/wiki/Molten-Salt_Reactor_Experiment

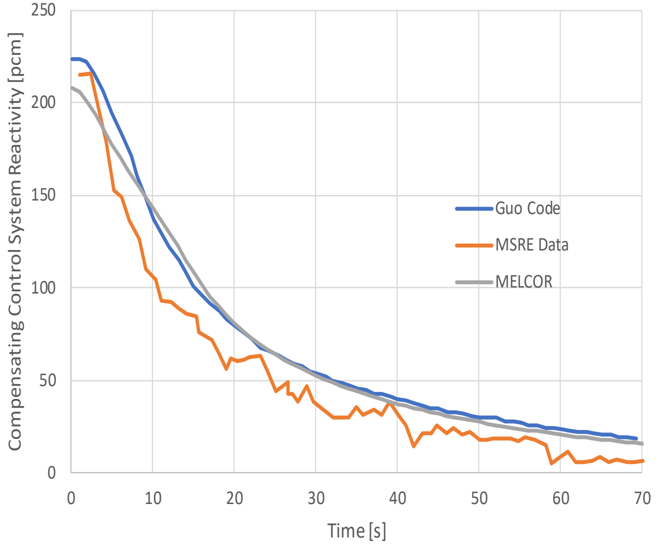
Control

- Fuel point kinetics – Derived from standard PRKEs and solved similarly
  - Feedback models
    - User-specified external input
    - Doppler
    - Fuel and moderator density
    - Flow reactivity feedback effects integrated into the equation set

$$\frac{dP(t)}{dt} = \left(\frac{\rho(t) - \beta_{eff}}{\Lambda}\right) P(t) + \sum_{i=1}^{6} \lambda_i C_i^C(t) + S_0$$

$$\frac{dC_i^C(t)}{dt} = \left(\frac{\beta_i}{\Lambda}\right) P(t) - \left(\lambda_i + {}^{2}/_{\tau_C}\right) C_i^C(t) + \left(\frac{V_L}{V_C}\right)\left(\lambda_i + {}^{2}/_{\tau_L}\right) C_i^L(t),$$
$$i = 1 \dots 6$$

$$\frac{dC_i^L(t)}{dt} = \left(\frac{V_C}{\tau_C V_L}\right) C_i^C(t) - \left(\lambda_i + {}^{1}/_{\tau_L}\right) C_i^L(t),$$
$$i = 1 \dots 6$$



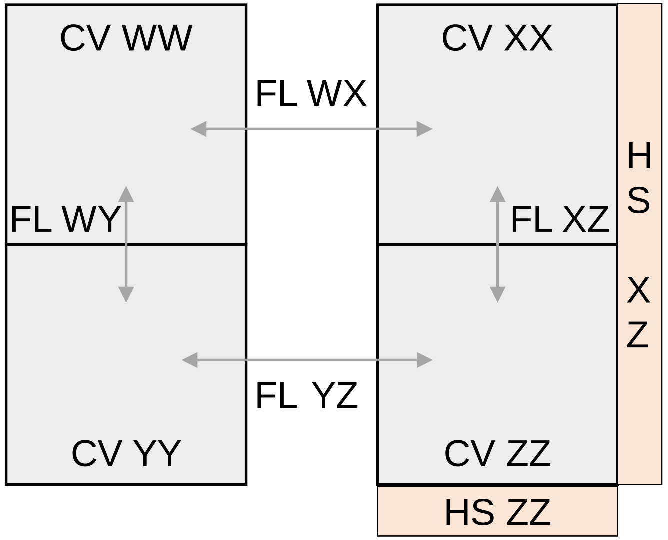
- Transmutation – Depletion Module (under development)
  - Treats transmutation of the initial radionuclide inventory (radioactive decay and neutron interactions) during severe accidents including mass transfer between radionuclide classes

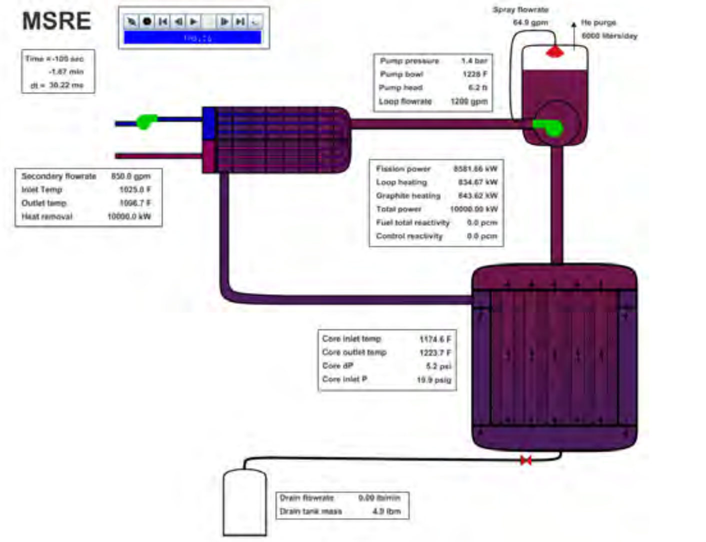
$$\frac{dN}{dt} = \left(A_\lambda + A_\phi \Phi\right) N(t) + S(t)$$

- $N(t)$: vector of isotope number densities
- A_λ: radioactive decay transition matrix
- A_ϕ: neutron interaction transition matrix
- Φ: scalar neutron flux
- $S(t)$: eternal isotope source

Cool

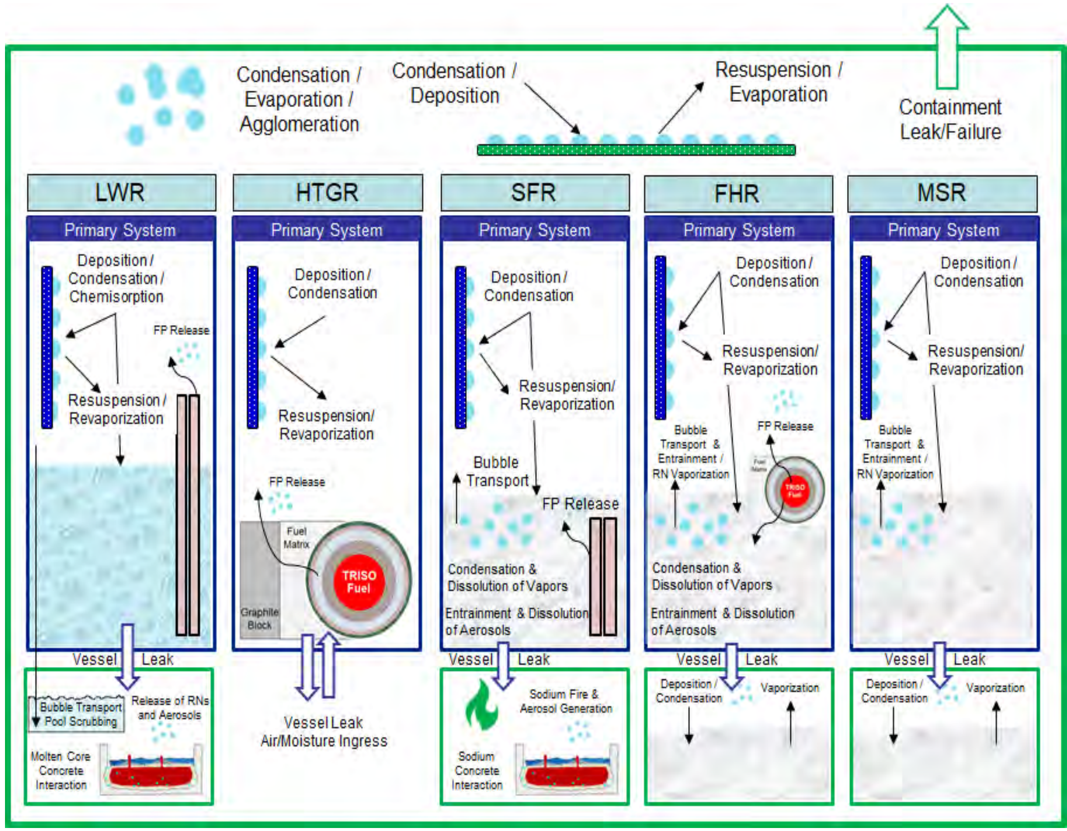
- Generalized EOS – Equations of state for multiple working fluids are presently available in MELCOR including water, sodium, and FLiBe.
  - MELEOS (under development) can generate equations of state for any fluid with the necessary data
- Thermal hydraulics – CVH/FL Packages
  - The CVH package defines control volumes (CV)
  - The FL package defines flow paths (FL)
- Heat Transfer – HS/CVH/COR Packages
  - The HS package defines heat structures (HS) that model radiative and conductive heat losses
  - The CVH package manages convective heat losses
  - The COR package controls heat losses of heat bearing and other core structures



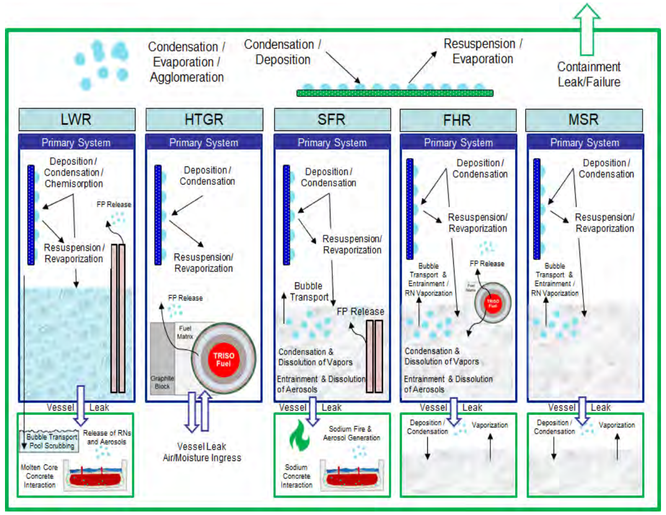


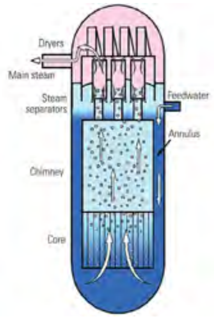
Contain

- Generalized Radionuclide Species – DCH/RN1
  - Default 17 representative radionuclide species/elements (RN classes)
  - Users have the ability to redefine/add RN classes
  - Radionuclide species are categories of chemically similar (similar in transport and retention mechanisms) radioactive elements/compounds
  - Each radionuclide species is representative of a set of elements and the corresponding collapsed isotopic masses
  - MELCOR does not currently model RN class masses at the isotopic level or mass transfer between RN classes
- Generalized Radionuclide Transport and Retention (GRTR)
  - MELCOR treats transport and retention of RN classes by various physiochemical processes in vapor and aerosol form by default; including aerosol size distribution (called "sections")
  - The GRTR model enhances these capabilities to allow for user-defined RN forms and subsequent formwise/sectionwise transfer between RN forms

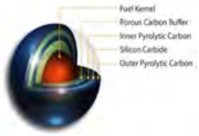


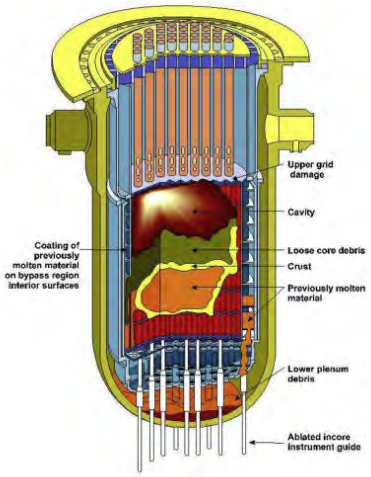
MELCOR Modeling Scope

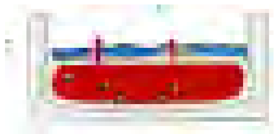




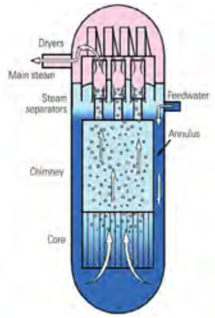
- Thermal hydraulics
- Fuel thermal-mechanical response
- Core degradation
- Ex-vessel damage progression
- Fission product release and transport
- Reactivity Effects







MELCOR Modeling Scope



Thermal hydraulics

MELCOR EOS

- Default Fluid: Water
- Implementation
  - Basis: Density-Temperature
  - Single phase: functional implementation (Keenan and Keyes)
  - Two-phase: pre-computed table of vapor dome values
- Properties:
  - Pressure (and derivatives with respect to the basis)
  - Internal Energy
  - Entropy
  - Enthalpy
  - Isochoric Heat Capacity

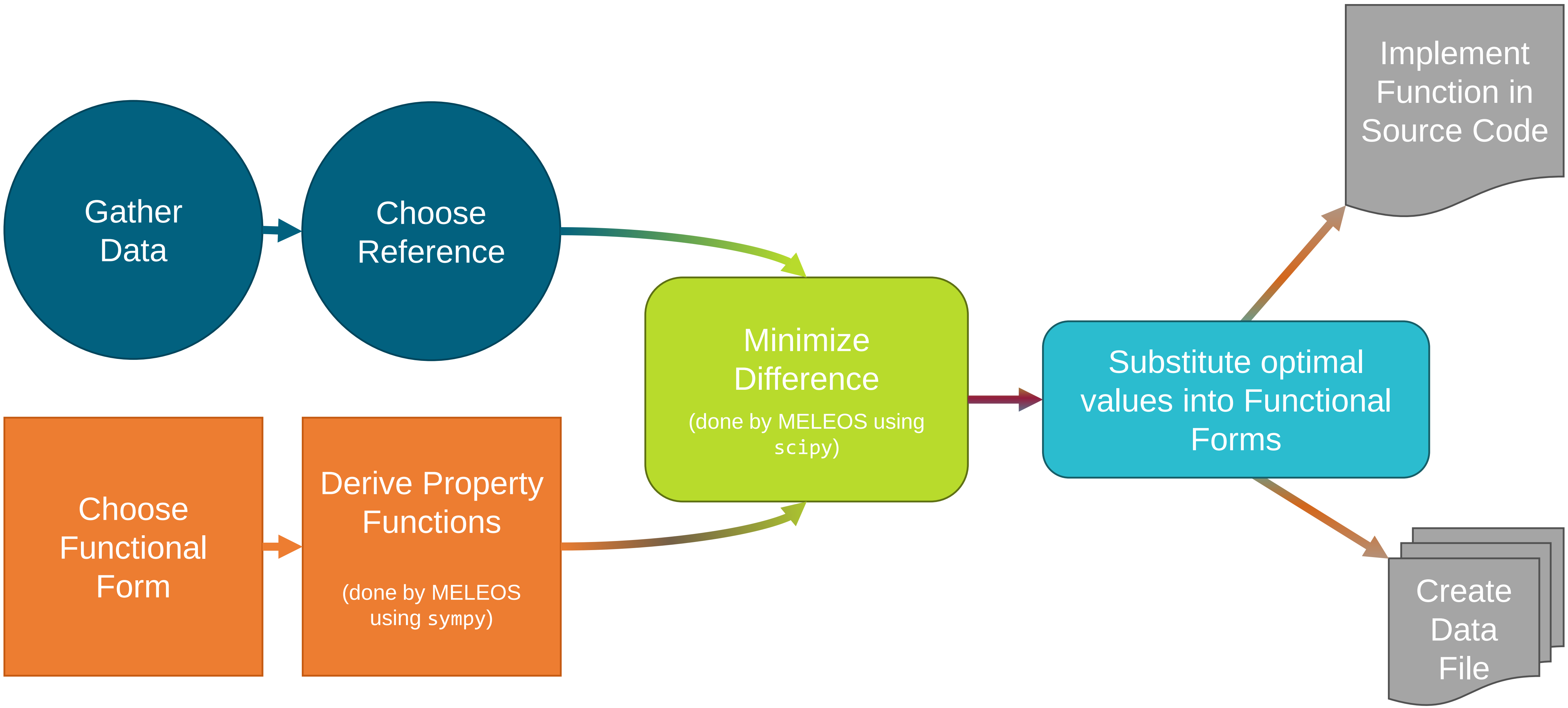
- Two Extensions
  - Sodium Chemistry Package
    - SIMMER EOS implementation
    - Function-based (no tables) for one- and two-phases
  - External file-read
    - Table-based EOS, cubic/linear interpolation
    - Requires viscosity, thermal conductivity, surface tension closures in codebase
    - Fluids:
      - Sodium
      - Lead-Lithium
      - FLiBe
      - … others

Helmholtz Potential

- A fundamental relation from thermodynamic theory
- Natural function of density and temperature
- Related to all thermodynamic variables
- Can be made accurate over the entire fluid range (liquid and gas phases)
- Differential definition of Helmholtz Free Energy f in terms of the entropy s, temperature T, pressure P, and volume v / density ρ
- $\mathrm{d}f = -s\,\mathrm{d}T - P\,\mathrm{d}v = -s\,\mathrm{d}T - P\,\mathrm{d}(1/\rho)$
- Integral definition of Helmholtz Free Energy f in terms of the internal energy e, temperature, and entropy
- $f = e - Ts$

- Helmholtz Relations
  - $P = \rho^2 \frac{\partial f}{\partial \rho}$
  - $e = -T \frac{\partial f}{\partial T} + f$
  - $s = -\frac{\partial f}{\partial T}$
  - $c_p = -T \frac{\partial^2 f}{\partial T^2} + \frac{\rho T \left(\frac{\partial^2 f}{\partial \rho \partial T}\right)^2}{\left[2\frac{\partial f}{\partial \rho} + \rho \frac{\partial^2 f}{\partial \rho^2}\right]}$ (Isobaric Heat Capacity)
  - $w^2 = \rho \left[2\frac{\partial f}{\partial \rho} + \rho \frac{\partial^2 f}{\partial \rho^2} - \rho \frac{\left(\frac{\partial^2 f}{\partial \rho \partial T}\right)^2}{\frac{\partial^2 f}{\partial T^2}} \right]$ (Isentropic sound speed)

MELEOS



Gather Data
Choose Reference
Choose Functional Form
Derive Property Functions
(done by MELEOS using sympy)
Minimize Difference
(done by MELEOS using scipy)
Substitute optimal values into Functional Forms
Implement Function in Source Code
Create Data File

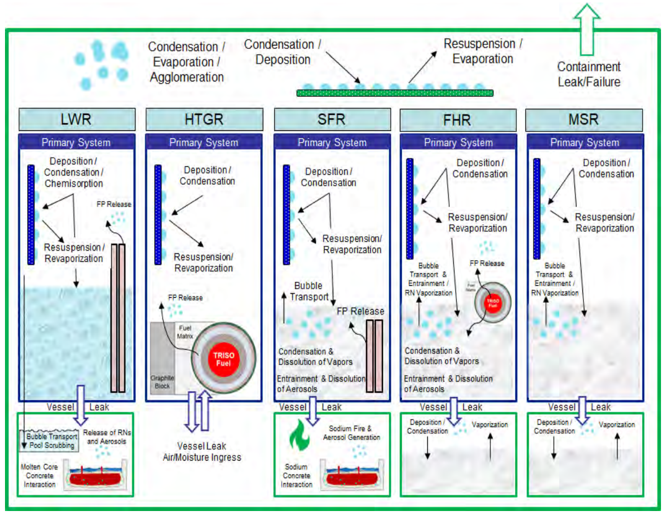
Next Steps

- Produce a binary external file for use with MELCOR
  - Make needed source code changes for non-thermodynamic data
  - Perform a demonstration calculation
  - Explore incorporating Helmholtz fit directly into source

- Gather other sources of data to improve current Chloride EOS
  - Sound speed is too low
  - Need variable pressure

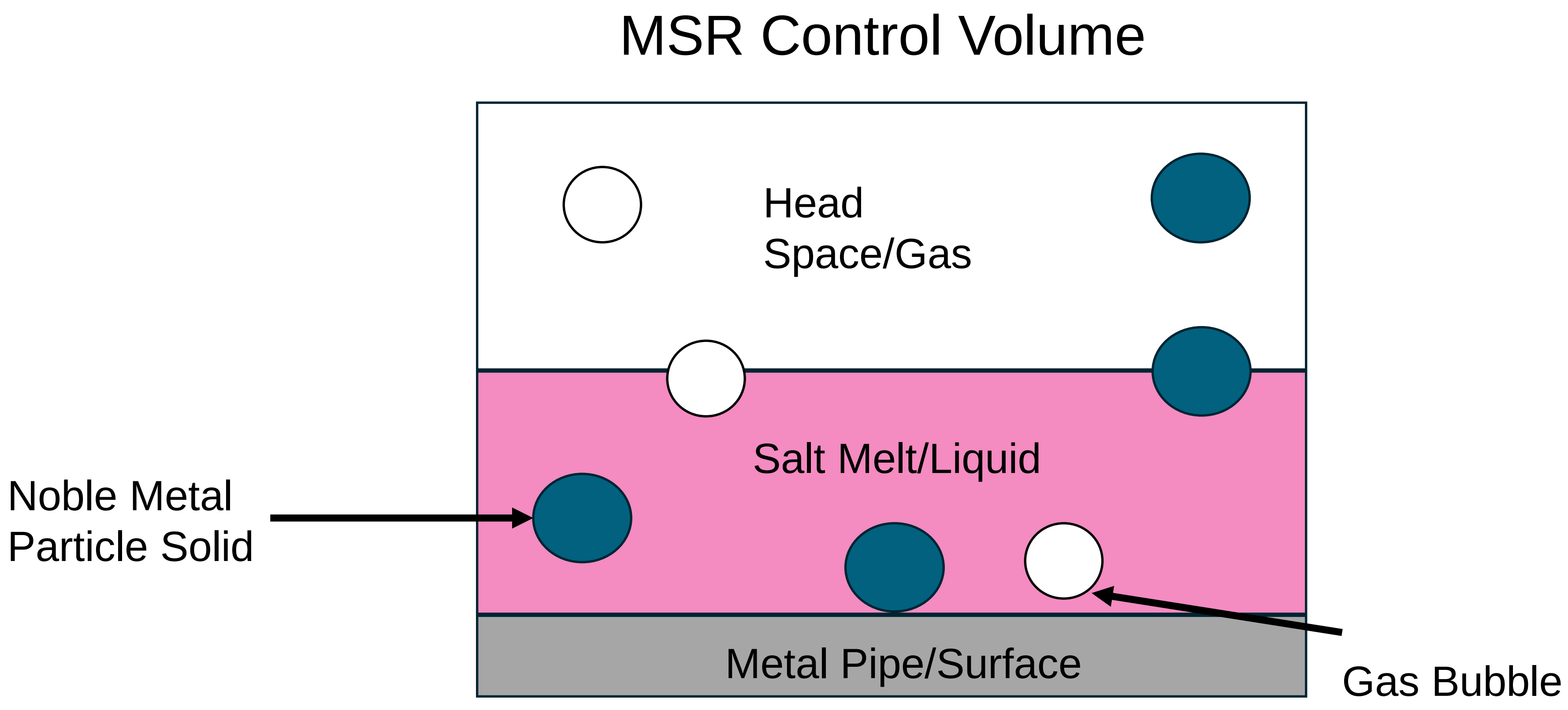
- Fit other salts and compositions using MELEOS for more applications

MELCOR Modeling Scope



Fission product release and transport

Control Volumes Must Account for All MSR Chemistry



Many different chemical processes can occur in one MELCOR control volume

Reactions are Chemical, Mechanical and Thermal Induced

- Chemical processes involve the transfer and interaction of electrons (bond breaking/making, surface adsorption)
- **Chemical Reactions:** oxidation/reduction, sublimate and bubble formation (decay to gas species), precipitation, adsorption
- Mechanical processes involve a physical force (gravity, pump spray)
- **Mechanical:** aerosolization (spray nebulization), bubble bursting, liquid splattering
- Heat processes involve the exchange of energy (temperature)
- **Thermal:** Melt, crystallization, gas condensation

Reactions and Speciation can be Characterized by Thermochimical Databases and Gibbs Energy Solvers

- Speciation within each MELCOR node could be handled by thermochemical databases (MSTDB-TC) coupled with a solver (Thermochimica)

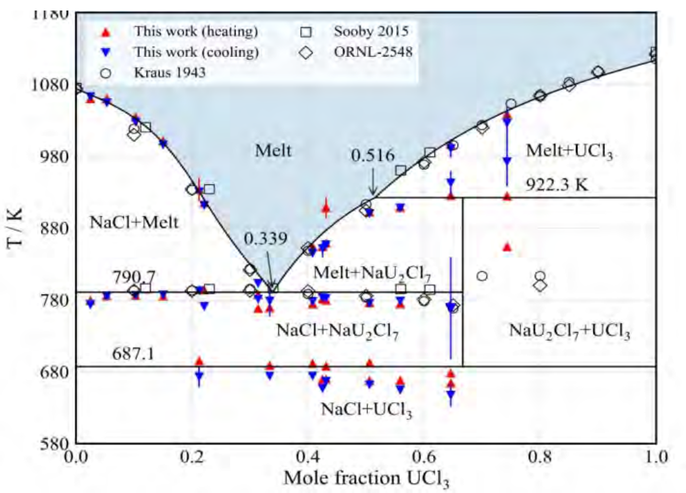
- Proof of concept demonstrated by Fred Gelbard for cesium

- Calling Thermochimica + MSTDB-TC for all MELCOR nodes for simulation duration would be expensive

Speciation can be simplified for MELCOR

Molten Salt Thermal Properties Database - Thermochemical
UofSC
MSTDB-TC

T. Besmann (UofSC)



Yingling et al., J Chem. Thermo 2023, 179, 105974

Application of MELCOR for Simulating Molten Salt Reactor Accident Source Terms

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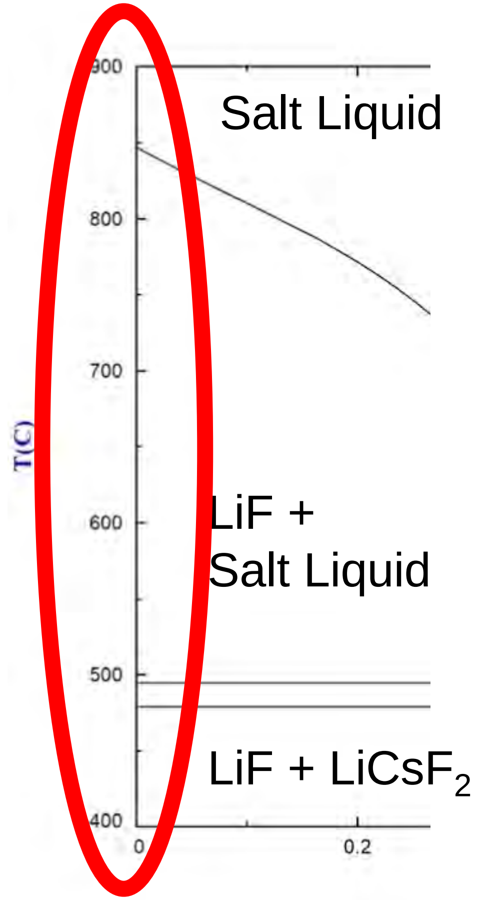
Nuc. Sci. and Engin 2023, 197, 2723-2741

Thermochimica
M. Piro (McMaster)

Radionuclide Masses Minimally Affect Bulk Salt Thermochimical Properties

- Carrier and fuel salt mass is thousands of kgs while radionuclides (RNs) will be a few kgs
- RNs will quickly form products related to phase speciation, having little affect on bulk properties
- RNs can be treated in system as atomic defects



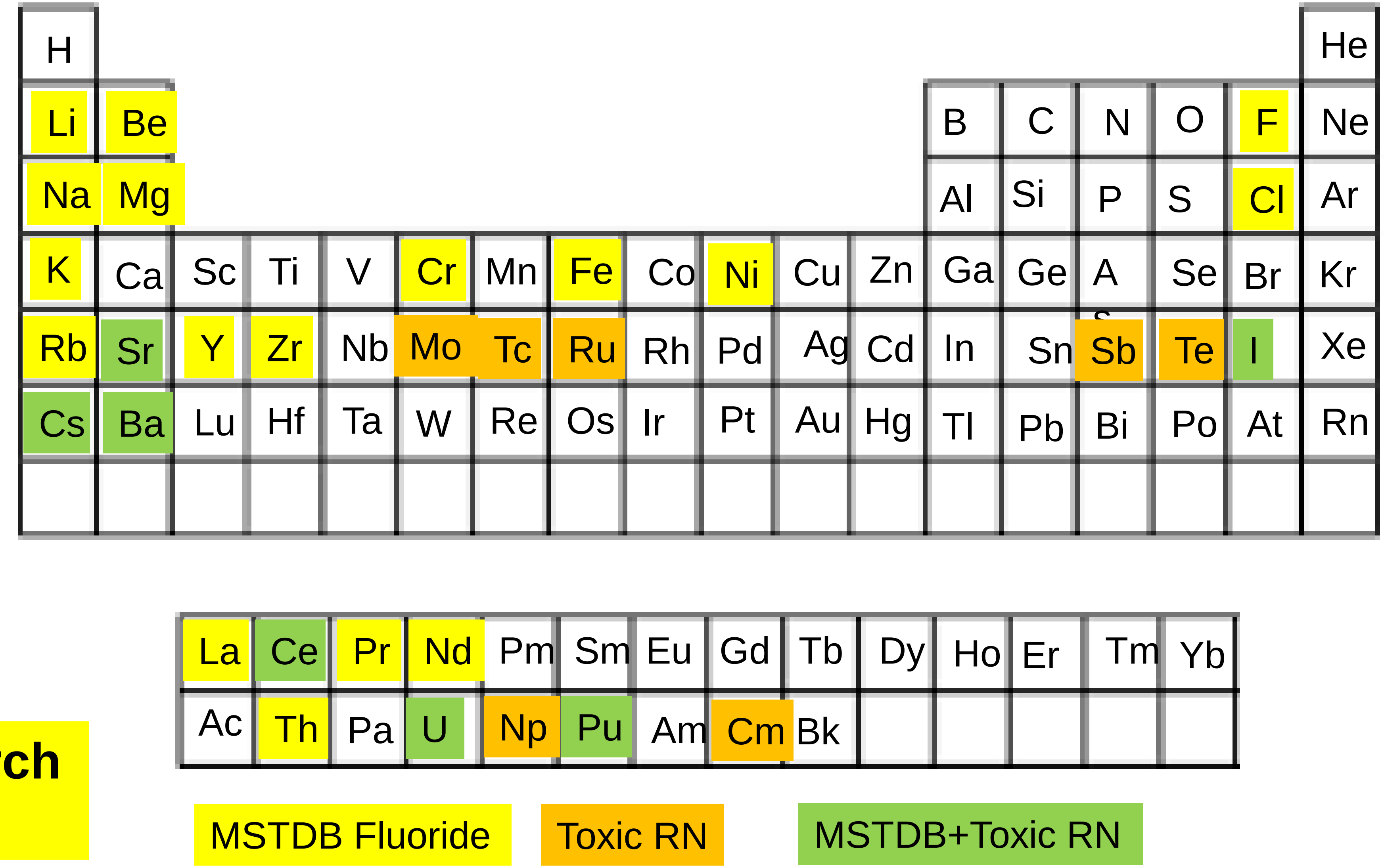
1% CsF mol frac with LiF

Technical report verifying assumption in process

Many Health-Consequence Systems Still Need Investigation

- Large focus has been on fuel salts and corrosion products
- Many fission product systems remain to be investigated
- Chemical and mechanical understanding of fission products is important

Broader Salt Research Needed



Future Directions for MSR Chemistry Modeling

- Integration of ORIGIN/SCALE with MELCOR for fission product inventory
- Continual development of salt equation of state for density, viscosity, heat capacity (Troy Haskins)
- Colloid transport and absorption model for noble metals
- Salt-Xe/Cs migration and absorption in graphite core
- Xe bubble formation, migration and bursting

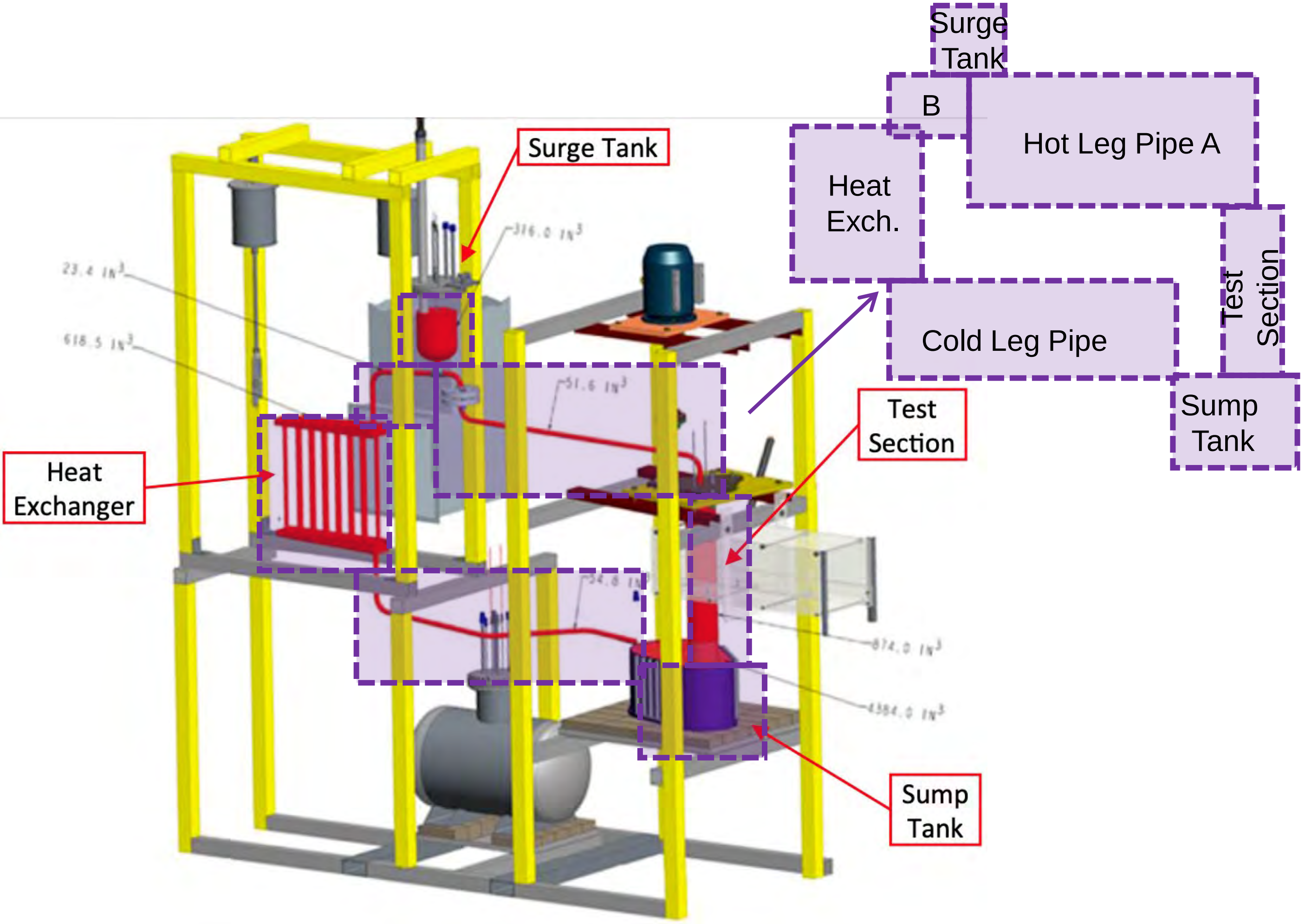
ORNL Liquid Salt Test Loop (LSTL)

- Test facility designed for measuring fluoride salt heat transfer inside a heated pebble bed.
- Incorporates a centrifugal pump to circulate FLiNaK salt.
- Inductive heating used to apply heat to the test section.
- Supporting loop infrastructure includes pressure control. trace heating system and instrumentation for salt flow, temperature, and pressure

LSTL in hood.

Yoder, G.L. et al., *High-Temperature Fluoride Salt Test Loop.* Oak Ridge National Laboratory. ORNL/TM-2012/430, 2015.

MELCOR MSR Model Demonstration Via LSTL

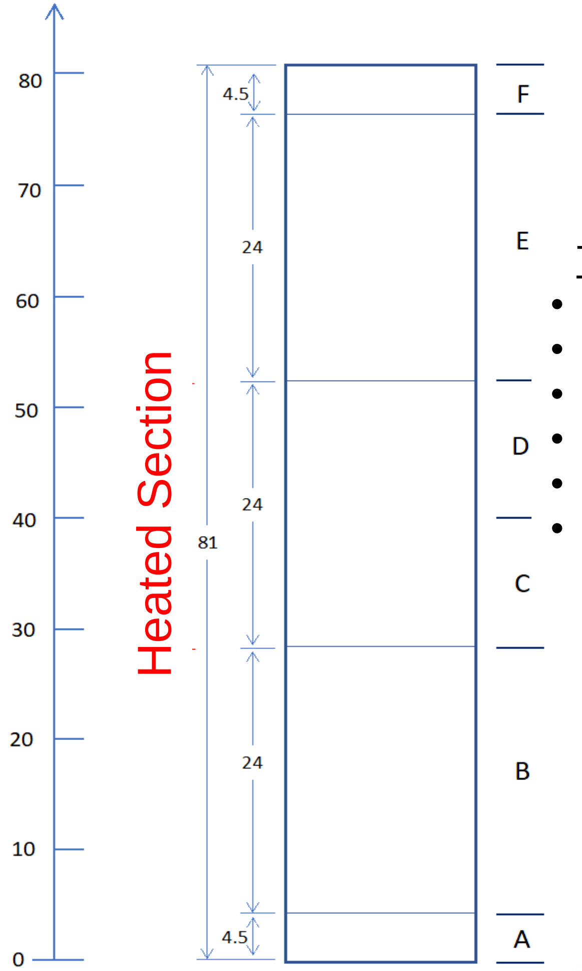


- MELCOR uses a collection of interacting and interconnected control volumes to model reactor flow paths, heat structures, etc.
- Work focuses on developing and demonstrating how MELCOR models can be used to model the steady state operation of LSTL
- Modeling Approach Details:
  - Liquid-salt-based coolant (but FLiBe instead of FLiNaK)
  - Heat-structure-based representation of Pebble Bed test section.
  - Testing of "in-development" MetaVolume approach in CVH to our standard approach.

From: *Avigni, Wysocki, and Yoder, "Liquid Salt Test Loop modeling using Trace", Annals of Nuclear Energy 106 (2017) 170-184*

Comparing 2023 and 2024 Experiments

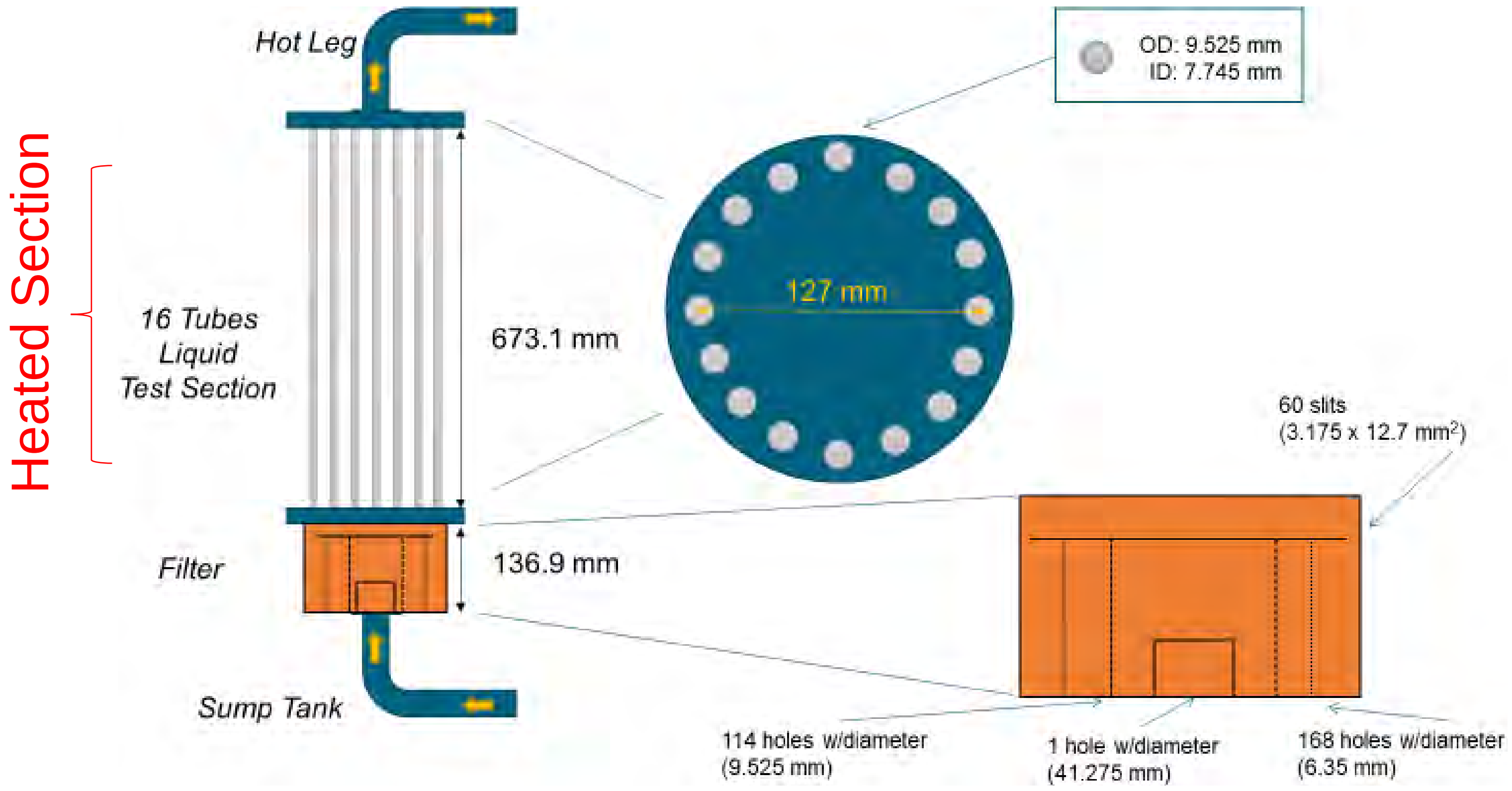
Pebble Bed (FY23)



Test Section Parameters

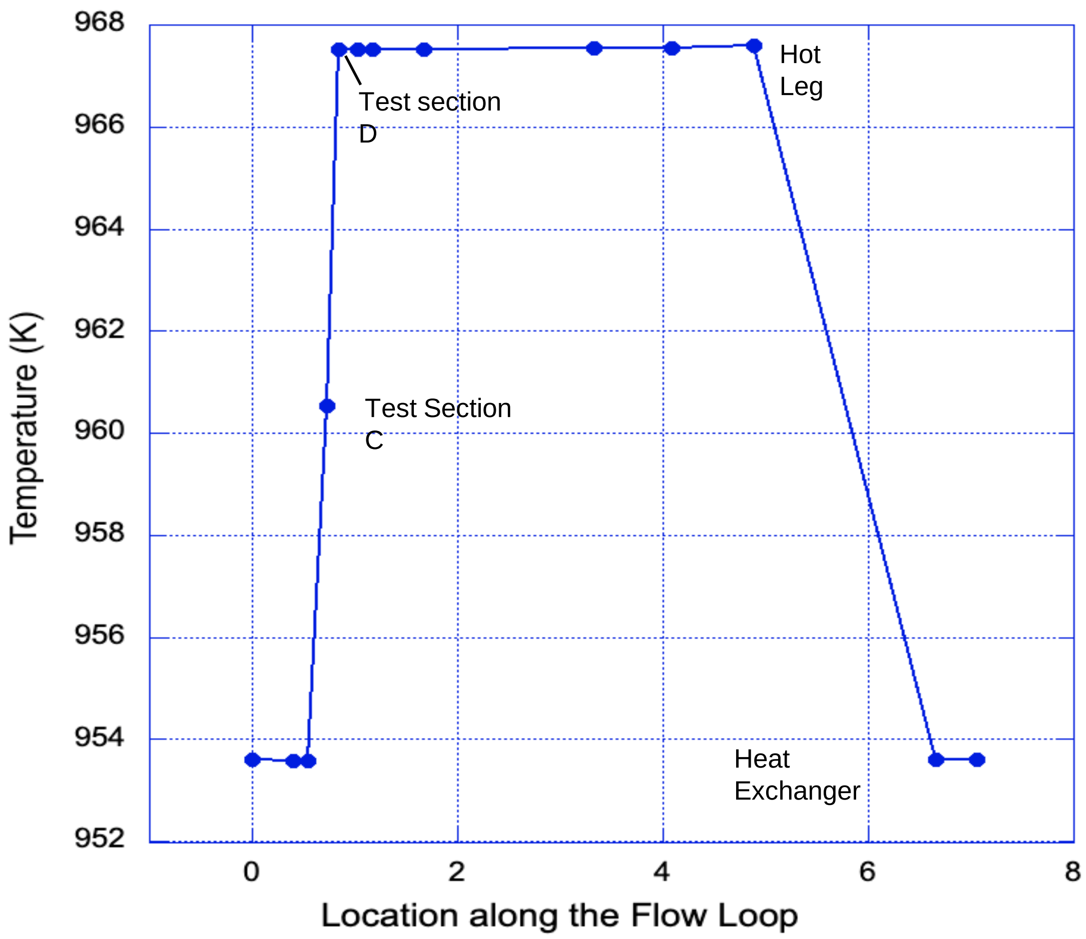
- 81 cm length
- 15 cm diameter
- 525 pebbles
- 3 cm in diameter
- 72 cm bed height
- 6 CVH control vols.

Liquid (FY24)

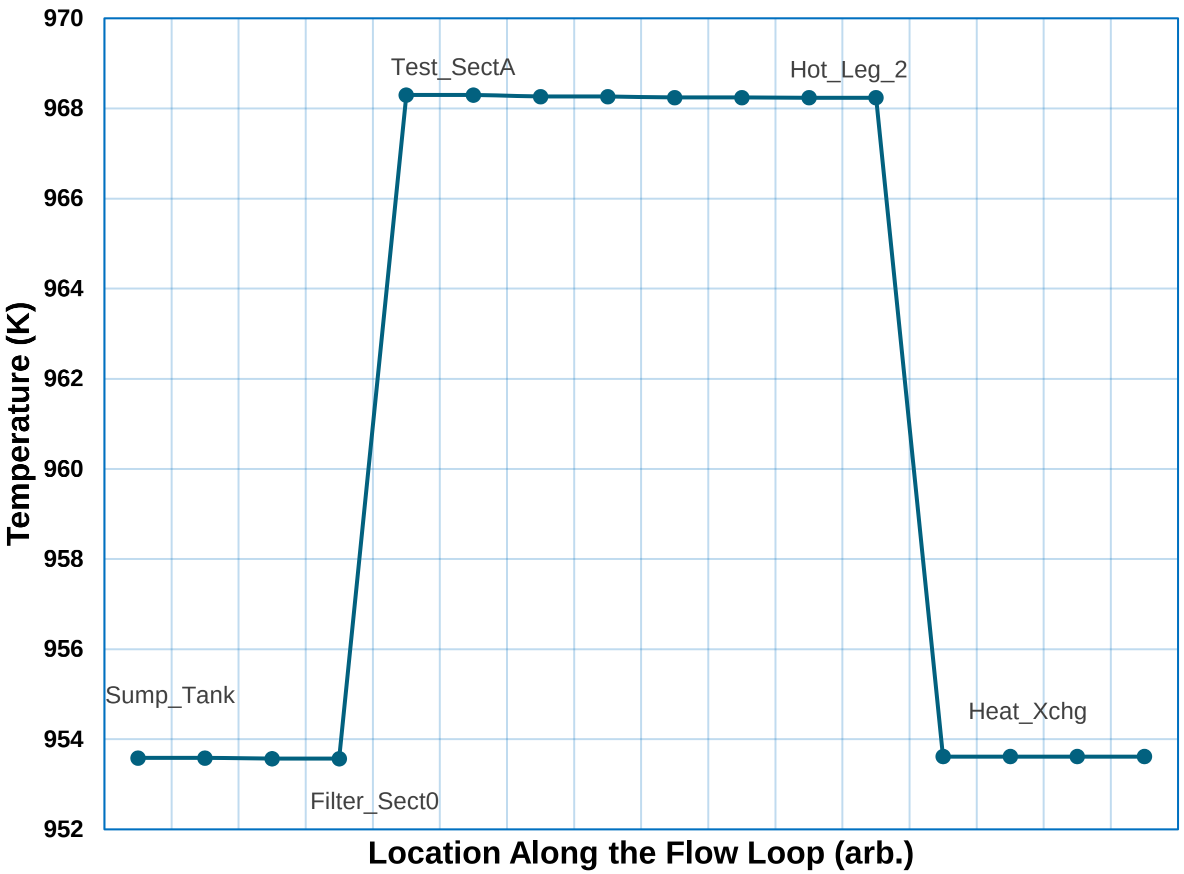


Experiments Have Different Heating Profiles

Pebble-Bed Test Section (FY23)



Liquid Test Section (FY24)



Future LSTL Modeling Work

- Improve heat exchanger model
- Acquire filter section physical measurements to improve model
- Implement a FLiNaK EOS in MELCOR
- Input new liquid test section model into MELCOR test suite

Summary

- MELEOS
  - A python package to develop equations of state for use by MELCOR is under development
  - This tool has significant capacity to support a broad range of current and upcoming MELCOR activities

- Radionuclide Transport
  - Simplified radionuclide chemistry models are being created from Thermochimica + MSTDB-TC calculations

- LSTL Model
  - Implemented different designs of LSTL for FY2023 and FY2024 experiments

Looking Forward

- MELEOS
  - Fit other salts and compositions using MELEOS for MSR mechanistic source term applications
  - Looking at incorporation of MSTDB data into MELEOS data via Saline and Thermochimica
- Radionuclide Transport Modeling
  - Continue to engage with partners to identify opportunities for MELCOR to develop transport correlations from both experiment and computational modeling
- LSTL Model
  - Continued verification of LSTL model
    - Implement FLiNaK as working fluid (dependent on MELEOS)
    - Etc.
  - Benchmark LSTL model with ORNL SAM model
  - Incorporate LSTL into validation matrix for MSR models as data becomes available

Acknowledgements

- Sandia MELCOR Team
- Ted Besmann/Juliano Schrone-Pinto and team (USC)
- Markus Piro (McMaster)
- Joanna McFarlane (ORNL)
- Patricia Paviet (PNNL)
- **YOUR NAME HERE**

WE WANT TO WORK WITH YOU!!!

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