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Model Refinement Studies for Molten Salt Freeze Port Conceptual Design Using COMSOL

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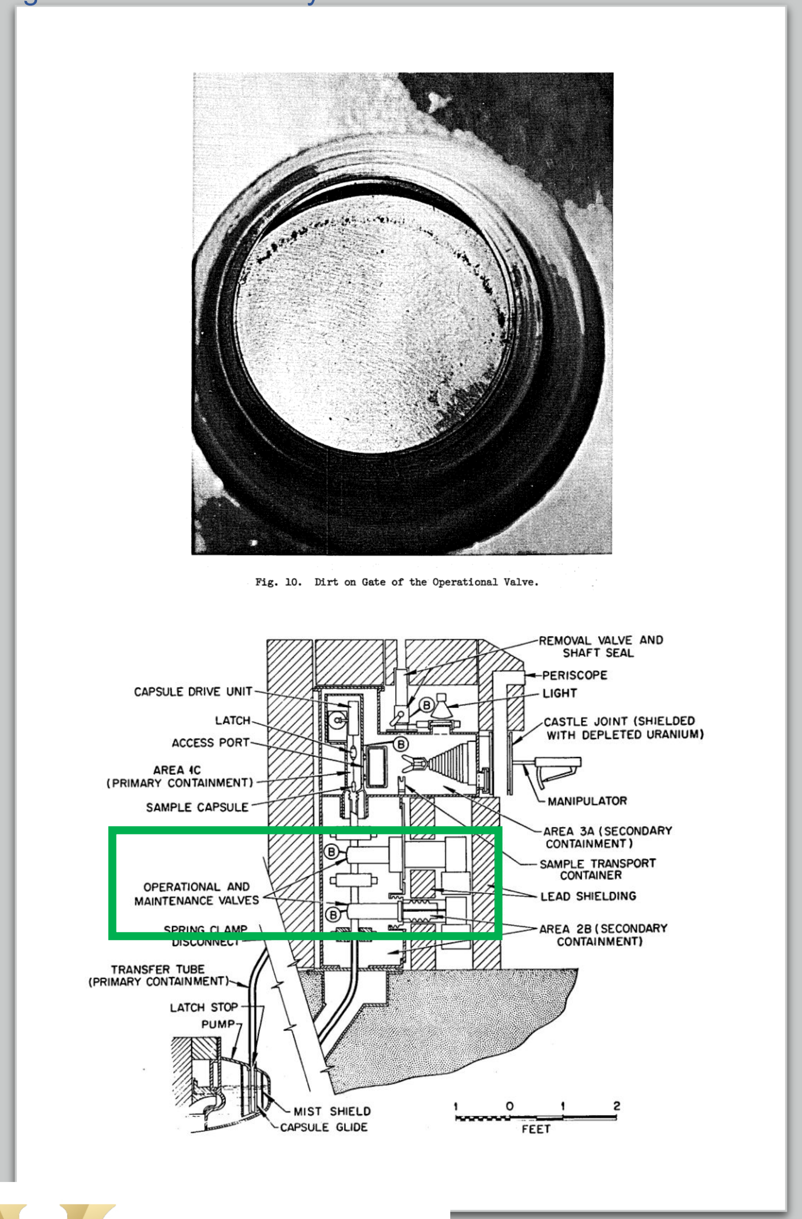
Introduction-Molten Salt Sampling

- MSRs are a type of advanced reactor concept being pursed as a viable alternative to carbon-emitting or intermittently-available renewable energy sources. MSRs are unique amongst advanced reactor concepts because:
  - Options for utilization of homogeneous liquid fuels that may offer improved safety margins
  - Higher outlet temperatures that can be used to support process heat applications such as hydrogen generation
- However, limited MSR operational experience and the sensitivity of reactor safety, safeguards, and operability to salt chemistry provide incentive for closely monitoring and controlling the salt composition within an MSR.
  - Salt characteristics of interest include redox potential, fissile material inventory, fission product speciation, and impurity concentrations
- In first-generation MSRs, this function is expected to be facilitated through isolating small samples of salt from the bulk salt volume for laboratory analysis

Image credit: Gallagher, R. (1971). ORNL-TM-3524, Operation of the Sampler-Enricher in the Molten Salt Reactor Experiment, Oak Ridge National Laboratory.



Introduction-Problems with Mechanical Valves in MSRs

- Within the Molten Salt Reactor Experiment (MSRE), a system called the Sampler-Enricher was used for salt sampling.
  - The system's exhibited numerous reliability issues that motivates its redesign for future MSRs.

- The Sampler-Enricher utilized electromechanical valves to isolate the primary salt system from the remainder of the Sampler-Enricher when not being used for sampling.
  - However, these valves exhibited operational difficulties:
    - Impacted travel of sample collection device within Sampler-Enricher
    - Improper sealing and leakage from surfaces encrusted with salt particles and corrosion products

- For this reason, Sampler-Enricher redesign efforts to-date have identified an alternative to traditional mechanical valves– the "freeze port."

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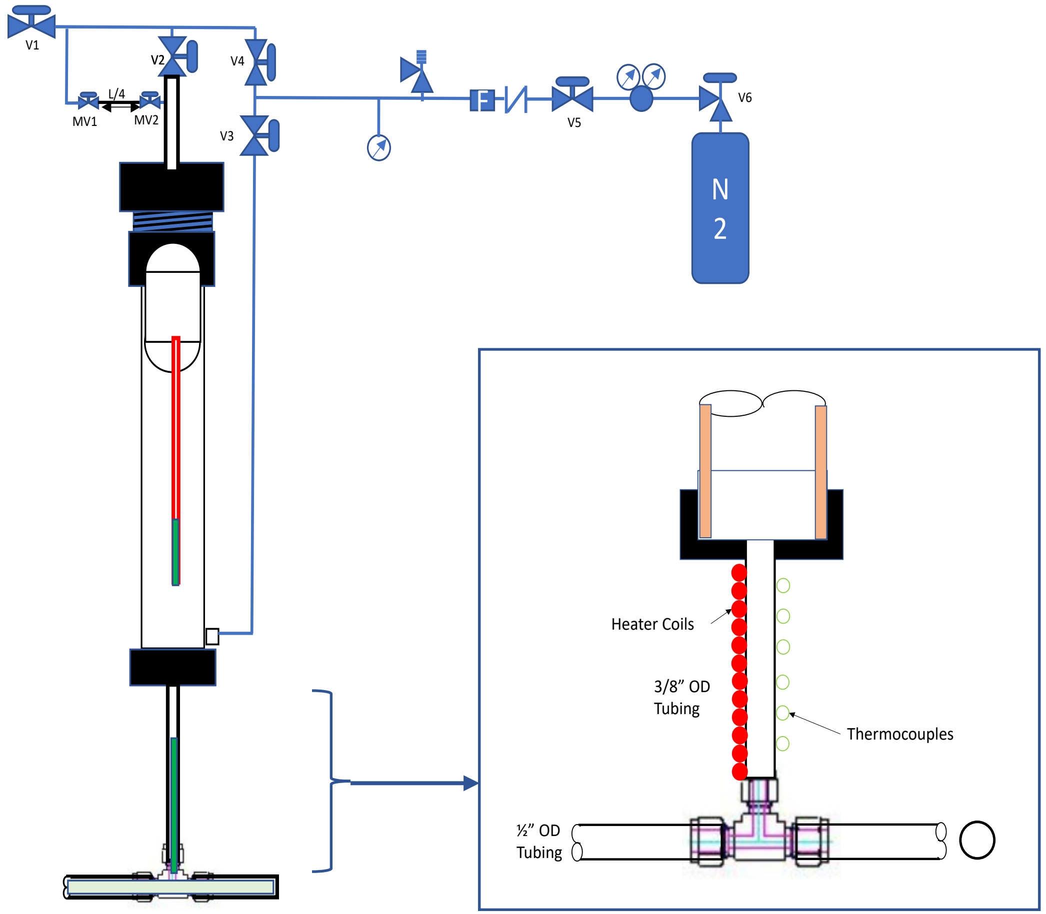
Introduction- Freeze Port Concept

- The freeze port is an alternative to a traditional mechanical valve that extends the freeze valves and freeze flange design concepts used within the MSRE.
    - Freeze valves and freeze flanges have also been considered by modern MSR designers.
- The salt within the freeze port is initially frozen, providing the same sealing function as a closed valve.
- When the salt in port is thawed (using external heaters), the port is considered open.
    - a sample collection device can be transported through the open salt to obtain a salt sample.
- Eventually the molten salt sampling system prototype (including freeze port) will be tested at the University of Michigan's FLUoride Salt Test FAcility (FLUSTFA).
    - However, the performance of the freeze port needs to be modeled prior to being tested in a molten salt environment.



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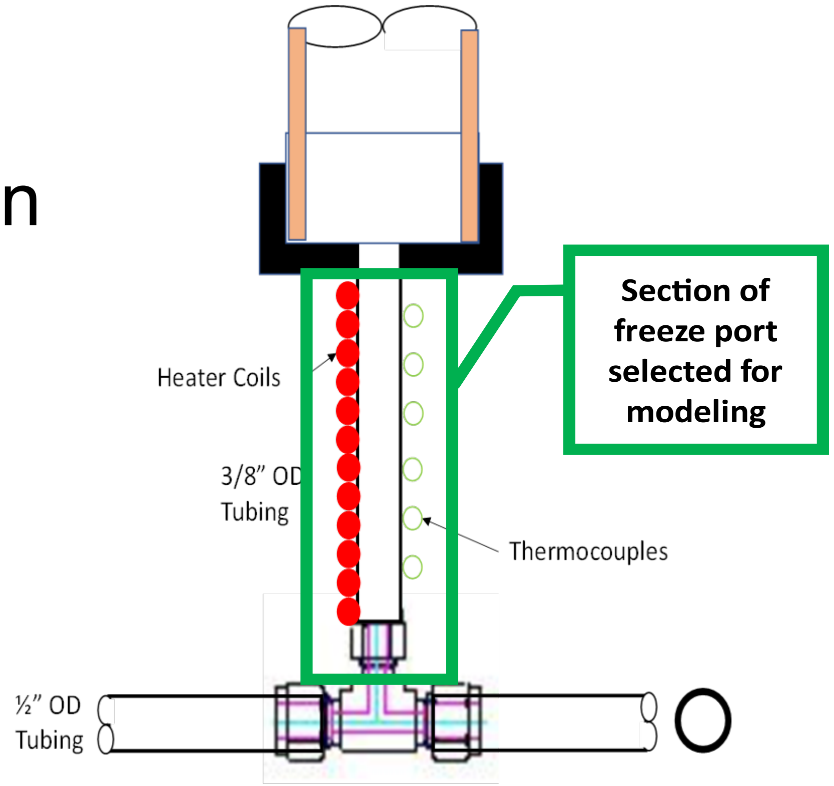
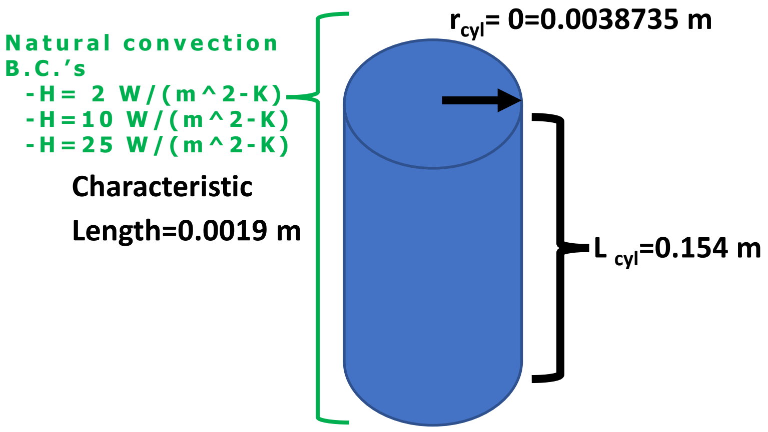
Questions to be Addressed by Heat Transfer Models

1. Can the freeze port be closed in a time that is somewhat comparable to what can be achieved by mechanical valves (<5 minutes)?

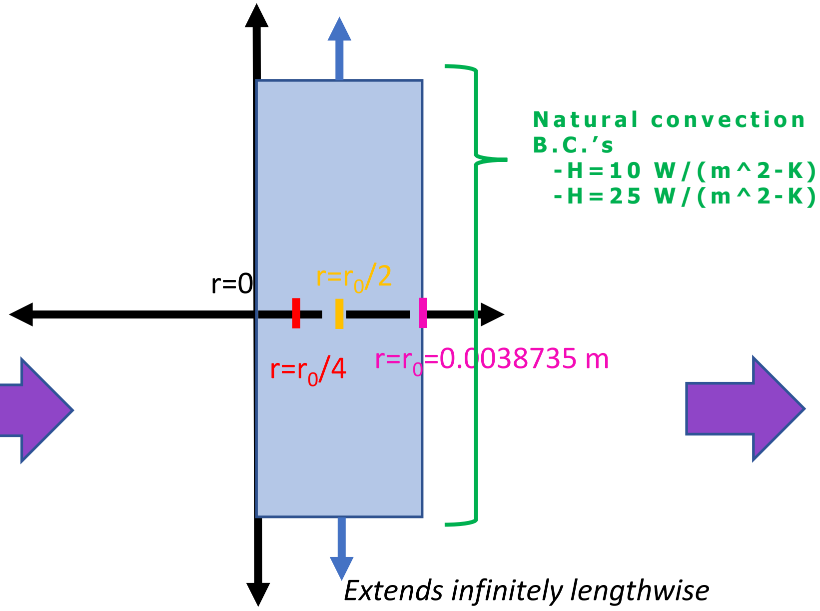
2. What happens to the freeze plug during temperature transients? Can the port remain closed?



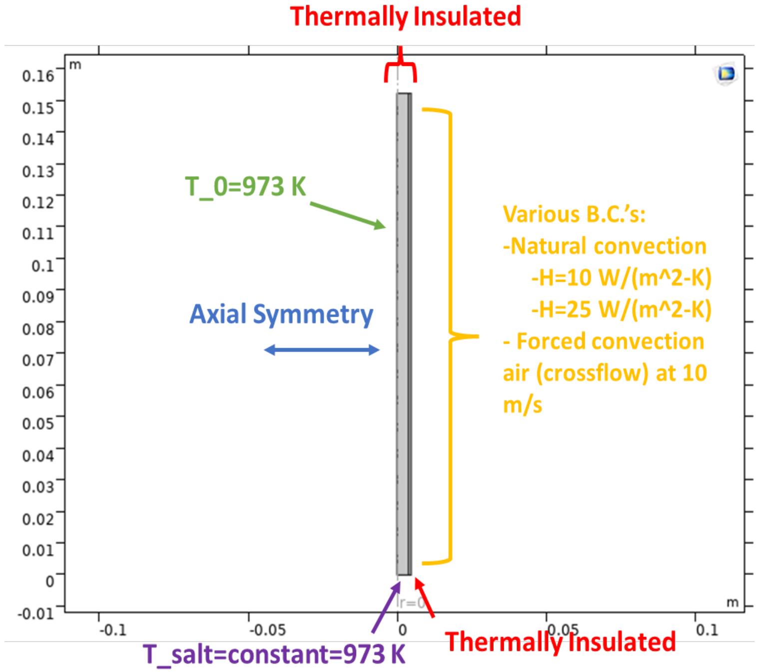
Modeling Approach



1. Analytical Solution Simplified Lumped Parameter



2. Refined Analytical solution to heat equation for semi-infinite cylinder exposed to external natural convection



3. Computational COMSOL model of phase change, including SS-316H piping, effects of latent heat, and temperature dependency of thermophysical properties

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Materials

- Models use the thermophysical properties of eutectic LiF-NaF-KF (FLiNaK), the salt used within FLUSTFA

Thermophysical Property	Value
Melting Temperature, T_{melt}	727.5 [K]
Latent Heat of Fusion, L_f	1.6E6 [J/kg]
Solid FLiNaK Density, ρ_s	2199.2 [kg/m^3]
Molten FLiNaK Density, ρ_l	2729.3-0.73(T), [kg/m^3]
Specific Heat Capacity, C_p	1906 [J/kg-K]
Thermal Conductivity, k_{th}	0.8024+0.00056(T-790) [W/m-K]

Apparent Heat Capacity Method for Modeling Phase Change

- COMSOL's default is to use the apparent heat capacity method for phase change modeling
- Stefan condition does not need to be solved for because melting/freezing front is implicitly tracked with modified specific heat capacity term (C_{app}) found with a user-defined half-width phase change interval, ΔT
- Over the phase transition interval, the properties of the material undergoing phase change are calculated as a weighted average of the solid and liquid properties dependent on the temperature at a given time step

P.D.E.'s

$$\frac{\partial T_l(\mathbf{x},t)}{\partial t} = \alpha_l \nabla^2 T_l(\mathbf{x},t);$$

$$\frac{\partial T_s(\mathbf{x},t)}{\partial t} = \alpha_s \nabla^2 T_s(\mathbf{x},t);$$

$$k_s \nabla T_s(\mathbf{x},t) - k_l \nabla T_l(\mathbf{x},t) = L_H \rho_s \frac{\mathrm{d}s(t)}{\mathrm{d}t}$$

$$\rho c_{app} \frac{\partial T(\mathbf{x},t)}{\partial t} = k \nabla^2 T(\mathbf{x},t)$$

Credit: M. Tiberga, D. Shafer, D. Lathouwers, M. Rohde, J.L. Kloosterman, Preliminary investigation on the melting behavior of a freeze-valve for the Molten Salt Fast Reactor, Annals of Nuclear Energy, 132:544-554 (2019).

Modified Specific Heat Capacity, C_{app}

$$c_{app} = \begin{cases} c_{pl} & T > T_m + \Delta T; \\ \frac{1}{\rho}(\theta_l \rho_l c_{pl} + \theta_s \rho_s c_{ps}) + L_H \frac{d\xi_m}{dT} & T_m - \Delta T < T < T_m + \Delta T; \\ c_{ps} & T_m - \Delta T \geqslant T, \end{cases}$$

$$\theta_l = \begin{cases} 1 & T > T_m + \Delta T; \\ \frac{(T - T_m + \Delta T)}{2\Delta T} & T_m - \Delta T < T < T_m + \Delta T \\ 0 & T_m - \Delta T \geqslant T. \end{cases}$$

$$\xi_m = \frac{1}{2}\frac{\theta_l \rho_l - \theta_s \rho_s}{\rho} \qquad \rho = \theta_s \rho_s + \theta_l \rho_l \qquad k = \theta_s k_s + \theta_l k_l.$$

Motivation for Model Refinement Studies

- COMSOL has been shown to require relatively high-resolution meshing to accurately capture phase change physics when using the apparent heat capacity method.
- The models are also sensitive to the choice of phase transition interval and time step (controlled by adjusting relative tolerance), as well as the interplay between these parameters.
  - If temperature change in a time step near the transition region is greater than the transition interval itself, COMSOL may neglect the latent heat, which results in significant temperature fluctuations.

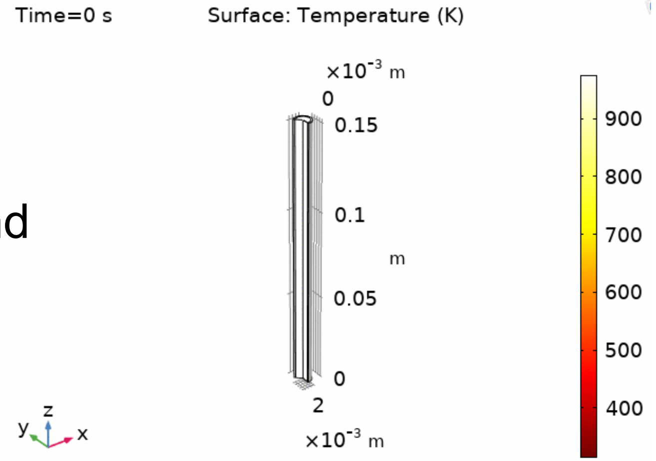
Parameter	Description	Values Used for Freeze Port Model	Values Found in Literature
ΔT	User-defined half-width of phase change transition interval	1, 2, 5, 10, 50 K	4 K [9] Values between 5-50 K [10]
M	Limitation on how large each mesh element can be (smaller maximum element size corresponds to larger number of mesh elements simulated)	1E-04, 3E-04, 5E-04	1E-3 m [9]
α	Convergence criterion- iteration stops when relative error is less than relative tolerance (in part responsible for size of time steps—COMSOL default is to use adaptive time stepping that is controlled by size of relative tolerance)	1E-04, 1E-03, 1E-02	1E-4 [10]

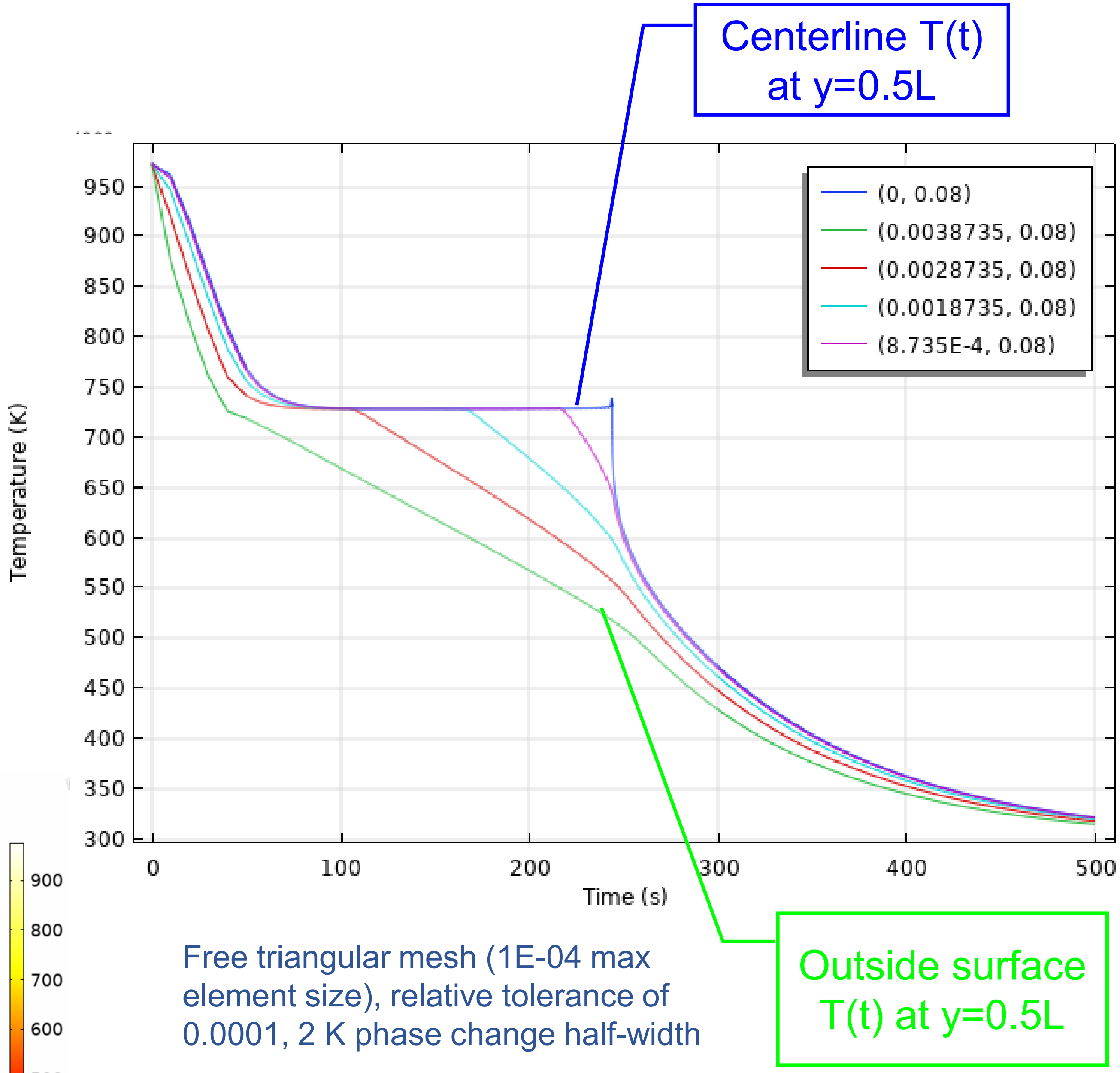
Results

- Analytical natural convection cooling solutions indicated that it would take between 150-200 seconds to approach phase transition temperature
  - Analytical solutions do not consider phase change
  - COMSOL models with H=25 w/(m^2-K) indicate that time required for freezing is likely unsupportive of operability and safeguardability goals for the design, prompting COMSOL investigations into the use of active cooling

- Using forced convection (10 m/s air at 297 K), freeze port can “close” in approximately 250 seconds (~4 minutes)

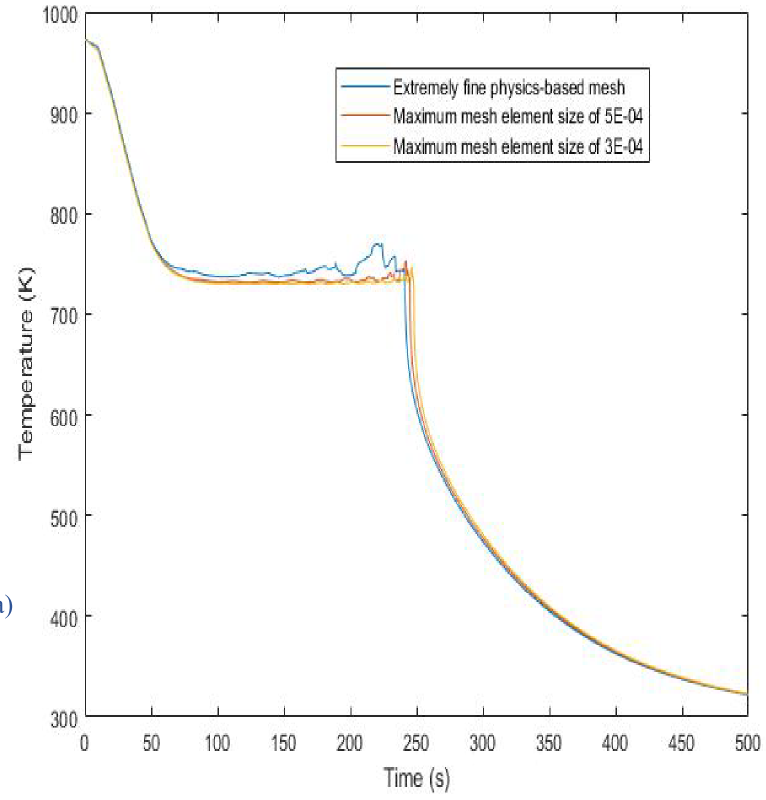
- Solution stability sensitive to mesh element size, relative tolerance/time step, and user-defined half-width of phase transition interval



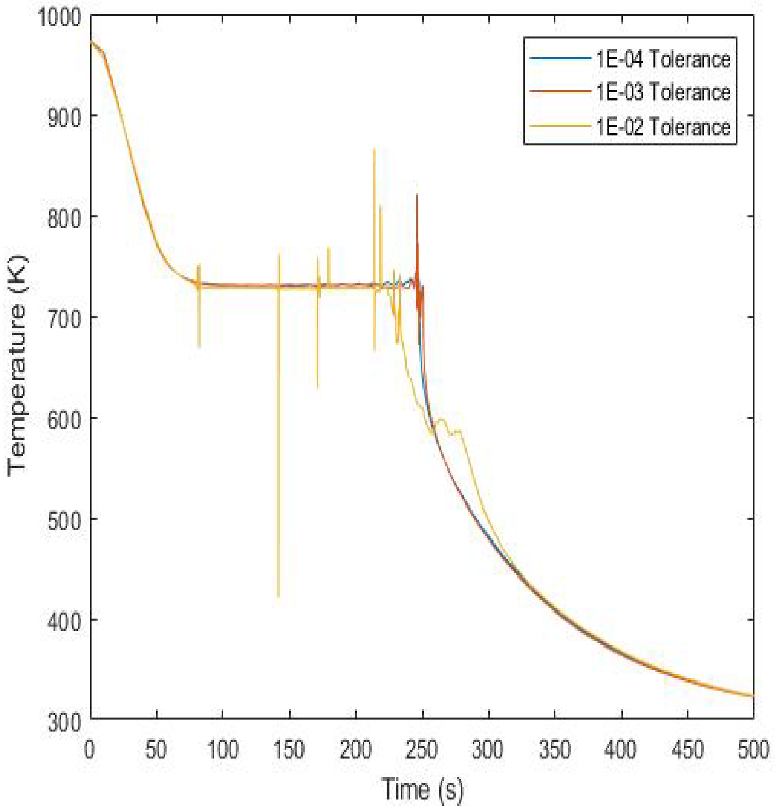


Free triangular mesh (1E-04 max element size), relative tolerance of 0.0001, 2 K phase change half-width

Refinement Studies: T(t)



a)



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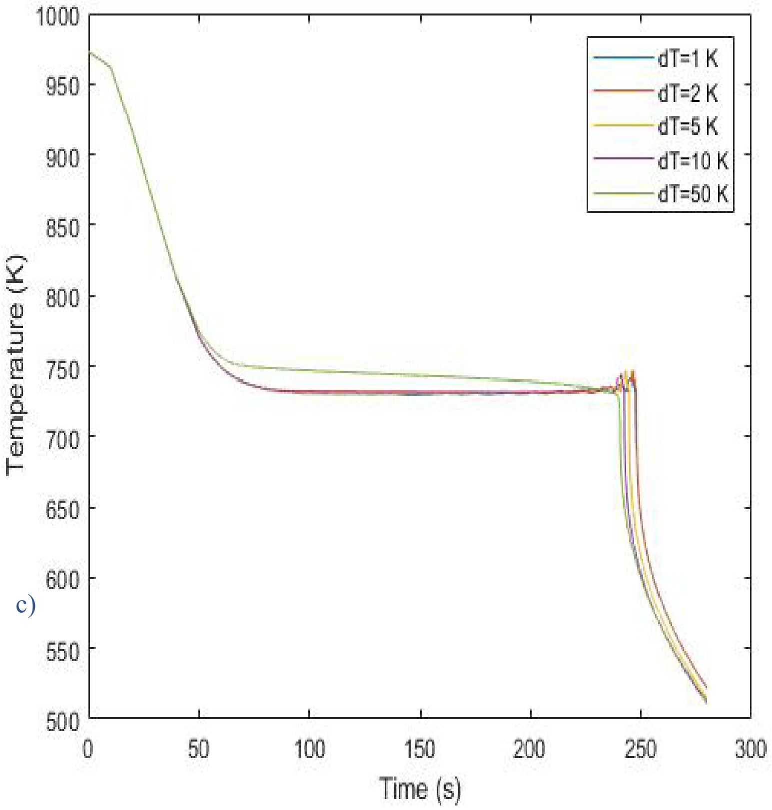

c)

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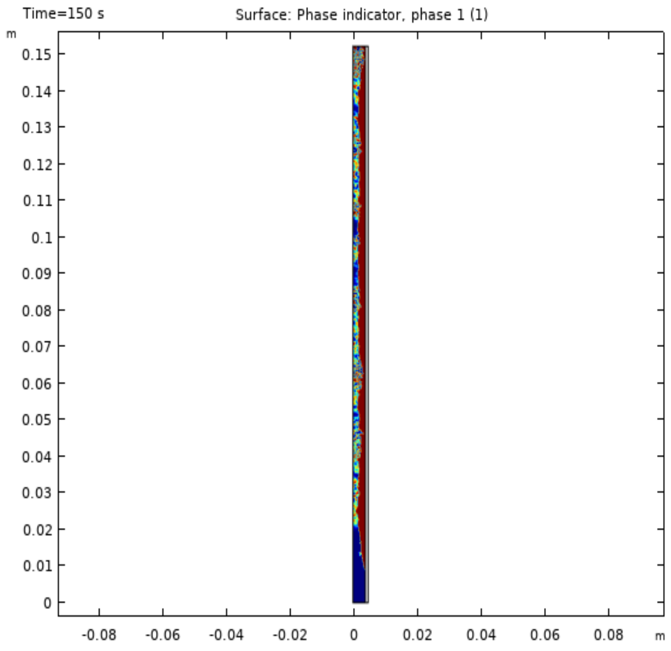
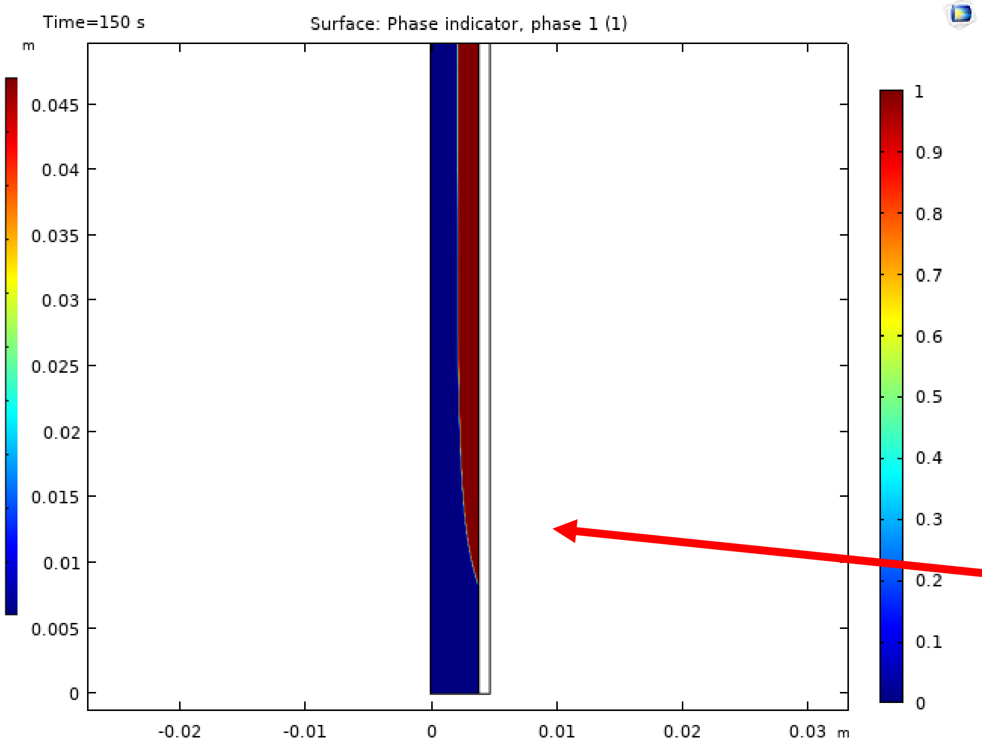
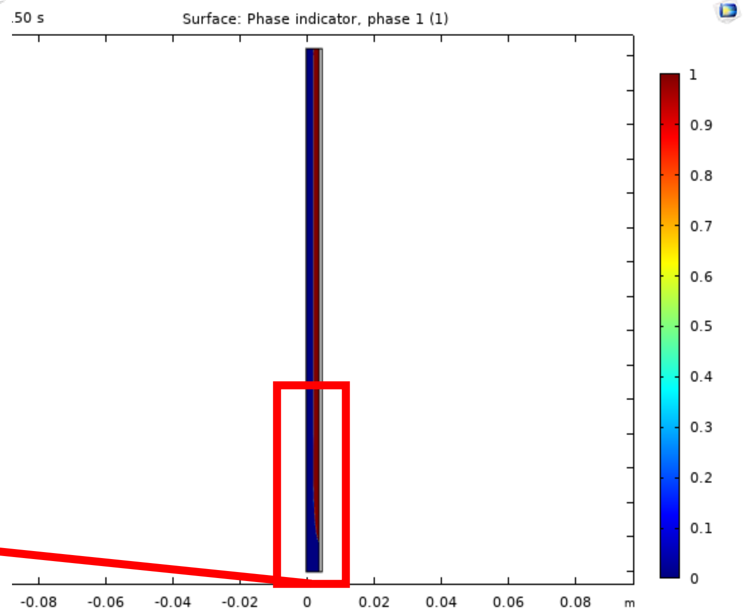
Refinement Studies- Phase Diagrams for Varying Tolerances

- Most significant numerical oscillations were due to the choice of relative tolerance.
  - Oscillations impact the "smoothness" of the transition from solid to liquid.
- For eutectic fluids, a smooth and sharp transition from solid to liquid is expected, and thus heterogeneities shown in 1E-02 and 1E-03 figures below are unrealistic



Relative tolerance=1E-02





Relative tolerance= 1E-04

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Solution Times for Refinement Studies

Mesh Parameters			Solution Times (s)
ΔT (K)	M (m)	α	
1	3E-04	1E-04	7249
2	3E-04	1E-04	4056
5	3E-04	1E-04	1388
10	3E-04	1E-04	631
50	3E-04	1E-04	575
2	1E-04	1E-04	44033
2	5E-04	1E-04	1004
2	3E-04	1E-03	4811
2	3E-04	1E-02	13721

Conclusions and Next Steps

- The initial refinement studies of the freeze port performance in COMSOL lend confidence to the component's ability to function as expected (i.e., close in a reasonably achievable time period) in a molten salt sampling system.
- Future studies using COMSOL will be performed using the simulation parameters identified during the refinement studies (as a starting point) to investigate:
  - Freeze port melting behavior and port opening times;
  - Freeze port behavior in off-normal scenarios, such as the event of loss of external cooling or a temperature increase in the primary salt below the port; and
  - Parametric sensitivity studies

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Questions or Comments?

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