Numerical analysis of Cl-based Molten Salt Spreading and Heat transfer using CFD-code

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1. Introduction

Molten Salt Reactors (MSRs) are gaining global attention due to their outstanding thermal efficiency and inherent safety features. In pursuit of carbon neutrality, MSRs are being developed for their capacity to provide high-temperature heat, which enhances electricity generation and supports industrial heating applications like high-temperature hydrogen production. This capability expands their use into Power-to-X (P2X) energy conversion systems.

MSRs use molten fluoride or chloride salts for fuel and as a primary coolant, reducing the risk of core meltdown accidents common in solid-fueled reactors. The high-temperature liquid fuel in MSRs has favorable negative reactivity coefficients because of density changes with temperature, which enhances their passive safety features without the need for active intervention systems [1-3].

For MSR commercialization, regulatory approval demands thorough safety assessments grounded in reliable experiments or numerical analyses [4]. Among the potential accident scenarios, salt spill accidents are critical as they could release fission products into containment structures and the environment. These accidents involve the leakage of molten salt from the primary circuit boundary, interacting thermally and structurally with adjacent components. Although the high melting point of molten salts indicates quick solidification upon leakage, restricting radionuclide mobility, accurate characterization of spreading behavior, cooling kinetics, and solidification dynamics are essential for radiological consequence analyses. Figure 1 shows a schematic representation of potential scenarios from a molten salt leak [5].

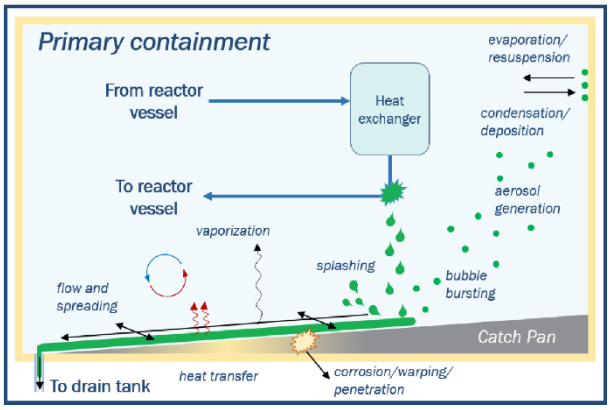

Fig. 1. A schematic of salt spill from the MSR primary loop onto the catch pan

The understanding of molten salt behavior during spill accidents is limited due to insufficient operational experience and experimental data. Molten salt reactors (MSRs) are still not commonly used in commercial applications. Significant research has been conducted at Argonne National Laboratory, where experiments with $NaCl$-UCl_3 salt mixtures and computational studies analyzing the spreading dynamics of FLiNaK salt were carried out using the one-dimensional MELTSPREAD code[6,7]. These investigations have provided essential insights and underscore the need for more sophisticated three-dimensional computational fluid dynamics (CFD) methods to capture intricate multiphysics phenomena better.

Numerical simulations of molten salt spill accidents present significant challenges due to the multiphase flow interactions between salt and ambient gas and the coupled heat transfer mechanisms, including thermal radiation and phase-change phenomena during solidification. The accuracy of these simulations critically hinges on selecting and parameterizing physical models, such as interface tracking algorithms, solidification formulations, turbulence closure schemes, and radiation heat transfer approximations. Evaluating the sensitivity of simulation outcomes to these model selections is essential for developing reliable analytical methods for MSR safety assessments.

This study uses CFD code to assess the sensitivity of various numerical models for simulating molten salt spreading and solidification phenomena during salt spill accidents. The Volume of Fluid (VOF) model with Continuum Surface Force (CSF) method for interface tracking, the Enthalpy-Porosity method for solidification modeling, Reynolds-Averaged Navier-Stokes (RANS) formulations for turbulence representation, and the Discrete Ordinates (DO) method for radiation heat transfer calculations are used. Through parametric analysis of significant factors such as mushy zone parameters, mesh resolution, turbulence model, and radiation angular discretization, this research establishes a numerical method for simulating molten salt behavior during salt spill accidents, enhancing the safety assessments for MSR systems.

2. Numerical method and boundary condition

2.1. Geometry and boundary conditions

Molten salt, made up of NaCl, KCl, and UCl_3, was spilled through a 5 mm radius inlet for 1,500 seconds at a temperature of 923 K and a flow rate of 2.2 cc/s. The boundaries of the top and side outlets feature 300 K air to facilitate natural circulation, while a convective heat transfer coefficient of 10 W/m²K was applied to the substrate's bottom. These conditions are detailed in Table 1.

Table 1. Boundary conditions of molten salt spreading numerical simulations

Spill condition	**Values**
Salt composition	NaCl-KCl-UCl_3
Initial salt temperature	923K
Corresponding spill mass	10.05kg
Volumetric flow rate	2.2cc/s
Corresponding mass flow rate	0.0067kg/s
Spill duration	1,500s
Substrate material	Steel
Substrate thickness	6.35mm
Radius of spill jet	5mm

Within ANSYS-Workbench's ANSYS-SpaceClaim, a steel substrate 500 mm in radius and 6.35 mm in thickness was created, while the fluid domain height was configured to 150 mm. Figure 2 shows the molten salt spilled from the substrate's center. A two-dimensional axisymmetric model was utilized. To reduce the impinging jet effects caused by the molten salt leaking onto the substrate, an inlet with a 5 mm radius was added, positioned at a height of 10 mm.

Using this geometry, a structured quad mesh was created in ANSYS ICEM CFD, with the mesh near all wall boundaries ensuring a y^+ value above 30.

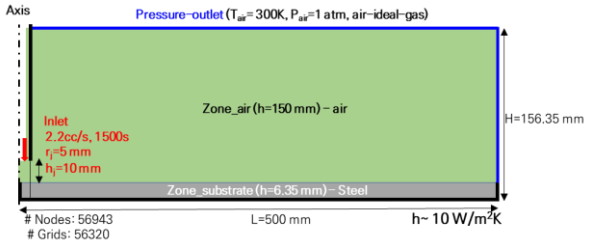

Fig. 2. Geometry of molten salt spreading numerical simulations

2.2. Thermodynamic Properties of the Molten Salt

To simulate the molten salt spill incident, the thermo-physical properties of NaCl–KCl–UCl_3 were analyzed using ANSYS Fluent. The thermodynamic properties of molten salt between 743K and 923K are outlined in Table 2 [8]. The density, specific heat capacity, thermal conductivity, and viscosity were defined through a piecewise-linear approach, ensuring linear variation in the liquid phase. Notably, the viscosity was modeled to increase by 2,000 times as the molten salt nears its solidification temperature. An absorption coefficient of 10,000 m^{-1} was applied for the radiative heat transfer from the molten salt to the surrounding air. Default properties from Fluent were used for air, with density adjusted according to temperature following the ideal gas law. A 144 kJ/kg latent heat was incorporated for heat transfer during phase transitions, including solidification or remelting.

Table 2. Thermodynamic properties of NaCl-KCl-UCl_3

Properties	**Values**
Melting point [K]	743.3
Density [kg/m^3]	3476 ~ 2875
Dynamic viscosity [kg/m·s]	10 ~ 0.001257
Specific heat [J/kg·K]	609.5 ~ 547.5
Thermal conductivity [W/m·K]	0.407 ~ 0.319
Latent heat of fusion [kJ/kg]	144
Surface tension [mN/m]	126.9 ~ 110.3
Radiation emissivity	1.0

2.3. Solver

Table 3 outlines the models and solver configurations applied to examine the spreading behavior and heat transfer mechanisms of the salt spill accident. The CFD analysis utilized ANSYS-Fluent 2024R1. The k-ω SST viscous model was selected as the major model due to its proven effectiveness in accurately predicting convection flows near walls and in free-shear environments. The generated mesh achieved y^+ values over 30 in all areas, and the standard wall treatment at the k-ε viscous model was applied to improve convergence within the viscous sublayer. The discrete ordinates (DO) model was selected for radiation heat transfer modeling, which included absorption, scattering, and reflection processes.

The PISO algorithm was employed for pressure-velocity coupling due to its convergence stability [9].

Table 3. ANSYS Fluent solver settings

Viscous model		SST k-omega
Radiation model		Discrete ordinates
Spatial discretization	Gradient	Least squares cell-based
	Pressure	Body force weighted
	Momentum	2nd order upwind
	Energy	2nd order upwind
Pressure-Velocity coupling		PISO
Multi-phase		Volume of fluid
Solidification & melting model		Enthalpy-porosity

The analysis involved a multiphase flow of air and molten salt. The Volume of Fluid (VOF) model was employed to capture the free surface flow and surface tension effects. Additionally, the enthalpy-porosity and Darcy friction models were used to calculate viscosity variations resulting from solidification and remelting, as well as phase change heat transfer and flow resistance.

2.4. Physics

The Volume of Fluid (VOF) model is a numerical method used to simulate multiphase flows and is especially effective at tracking interfaces between immiscible fluids. In this study, the Eulerian grid-based VOF approach was employed to calculate the fraction of fluids without needing to explicitly define the interface; instead, the volume fraction (α) in each cell indicates the fluid boundaries.

The key variable in the VOF model is the volume fraction, α, which describes the fluid fraction within a mesh. The mass and momentum conservation equations, which include the volume fraction, are presented as follows: Eq 1. [10]

$$\alpha = \begin{cases} 0, \text{ for a cell inside fluid a} \\ 1, \text{ for a cell inside fluid b} \\ 0 < \alpha < 1, \text{ for a cell inside transitional region} \end{cases} \quad (1)$$

$F_{surface}$ represents the surface tension force, modeled using the Continuum Surface Force (CSF) method. In this context, surface tension is connected to curvature and the surface tension coefficient. The equation computes variations in volume fraction over time as the flow evolves. Furthermore, Equations 4-5 demonstrate how the density and viscosity of the fluid mixture are obtained from the volume fraction, allowing for the simulation of interfacial physics and interactions. These equations define the fluid properties for each grid, accurately simulating the boundaries and interactions between the fluids.

$$\rho = \alpha\rho_1 + (1-\alpha)\rho_2 \quad (4)$$
$$\mu = \alpha\rho_1 + (1-\alpha)\mu_2 \quad (5)$$

ANSYS Fluent employs a Darcy friction model based on an enthalpy-porosity method to tackle these phenomena [9]. A liquid fraction (β) is defined for each cell: β = 0 signifies a fully solidified cell, β = 1 represents an entirely liquid cell, and values between 0 and 1 indicate a mushy zone where partial melting or solidification occurs. This liquid fraction is determined by the material's temperature and enthalpy, with total enthalpy being the sum of sensible heat (h) and latent heat (ΔH). The latent heat is calculated by multiplying the liquid fraction by the specific latent heat.

The energy equation defines the enthalpy of material as follows Eq 66.:

$$\frac{\partial}{\partial t}(\rho H) + \nabla \cdot (\rho \vec{v} H) = \nabla \cdot (k \nabla T) + S \quad (6)$$

The temperature resulting from the change in enthalpy corresponds to the liquid fraction. If the salt's temperature is below the solidification point, the liquid fraction equals 0. Conversely, if the salt's temperature exceeds the solidification point, the liquid fraction equals 1. For temperatures between the solidification and liquefaction points, follow Eq 7.

$$\begin{cases} \beta = 0 & T < T_{solidus} \\ \beta = 1 & T > T_{liquidus} \\ \beta = \dfrac{T - T_{solidus}}{T_{liquidus} - T_{solidus}} & T_{solidus} < T < T_{liquidus} \end{cases} \quad (7)$$

According to the enthalpy porosity model, the liquid fraction obtained from equation 7 is utilized in the flow resistance source term. Each cell's porosity corresponds to its liquid fraction. In fully solidified areas, porosity is zero, leading to a decrease in velocity. The momentum reduction resulting from the lowered porosity in the mushy region is described by Eq 8.

$$S = \frac{(1-\beta)}{(\beta^3 + \epsilon)} A_{mushy} \vec{v} \quad (8)$$

3. Results and discussion

The mesh sensitivity analysis of molten salt spill behavior utilized eight models with cell counts ranging from 11,320 to 112,884. A denser mesh reduced the spread radius due to improved resolution of molten salt-air interactions. For instance, the 11,320-cell mesh resulted in a spread radius of 268 mm, while the 112,884-cell mesh showed 253 mm, a 6% decrease.

The solidification model sensitivity was analyzed using mushy zone parameters from 10,000 to 500,000 kg/m·s. Lower values reduced flow resistance, increasing the spread radius by up to 52.8%. Accurate thermophysical properties or experimental validation are essential for optimal parameter selection. Heat transfer analysis revealed that lower mushy zone parameters led to higher heat removal and faster solidification rates.

Turbulence model sensitivity was evaluated using SST k-ω, Standard k-ω, and k-ε models. SST k-ω showed minimal error (<1%), while Standard k-ω differed significantly in heat removal and spread behavior after 400 seconds. Radiative heat transfer sensitivity using the DO model showed negligible differences (<0.05%) in spreading radius beyond 200 seconds but increased computational cost with higher resolutions.

These findings highlight the importance of mesh density, mushy zone parameters, turbulence models, and radiative heat transfer settings in accurately simulating molten salt spill behavior.

4. Conclusion

This study evaluated the sensitivity of numerical models for simulating molten salt spill behavior, focusing on mesh density, solidification parameters, turbulence models, and radiative heat transfer settings. Results showed that denser meshes improved resolution, while lower mushy zone parameters increased spreading due to reduced flow resistance. SST k-ω turbulence models provided reliable results with minimal error, and DO model sensitivity indicated negligible differences in spreading radius beyond 200 seconds but higher computational costs with increased resolution. These findings highlight the importance of optimal model selection and parameterization for accurate thermal-hydraulic simulations, contributing to enhanced safety assessments of molten salt reactors.

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