Preliminary analysis reflecting the radiation model under the two-phase system to simulate the solidification of spilled salt using OpenFOAM

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1. Introduction

Liquid-fueled molten salt reactors (MSRs) have been highlighted due to the unique advantages of their working fluid, a mixture of fuel and coolant salts. The working fluid provides high operating temperature without pressurization. The operating condition can increase the thermal efficiency of reactor and extend to usability to process heat such as hydrogen production.

In terms of safety, the high melting and boiling point of liquid fuel shows many advantages during transient situation. The high boiling point can remove the boiling crisis of primary system. In the ex-vessel condition such as salt spill, the high melting point can assure the rapid solidification of liquid fuel released from primary system. During a salt spill, the solidified fuel will retain the radioactive nuclides within it and decrease the environmental release. Consequently, the thermal properties of liquid fuel can increase the reactor safety during accident conditions. Despite of the guaranteed solidification, the release can occur through surface of spilled salt. Therefore, it is important to evaluate the spilled salt behavior.

Figure 1 shows the schematic of salt spill condition containing heat transfer and behavior of aerosol. The spilled salt transferred heat through conduction, convection and radiation. At the surface of the spilled salt, the vaporization and condensation can be occurred, and aerosol can be generated. These complex mechanisms affect the solidification and behavior of spilled salt.

Thus, the objective of the study is to develop a method for predicting heat transfer mechanism of spilled salt during salt spill accident using Computational Fluid Dynamics (CFD). The approach involves a comprehensive analysis of mass and heat transfer processes, the complex interactions between molten salt and its surroundings, and the phase changes of molten salt, which are crucial for understanding solidification and fluid dynamics.

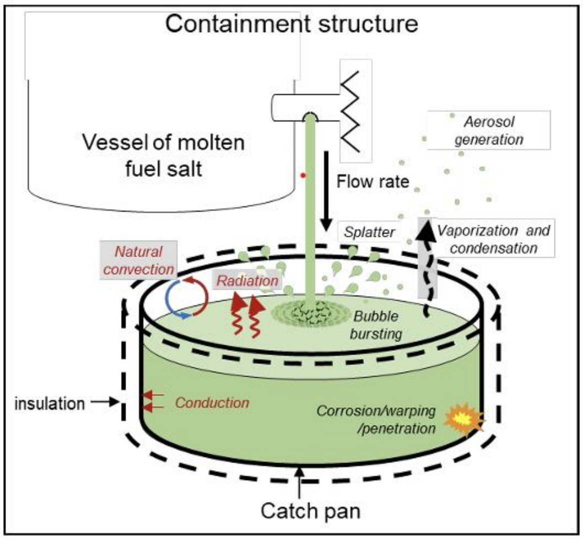

Fig. 1. A schematic of the heat removal process in a molten salt spill accident [1]

2. Numerical Methodology

2.1. Molten salt spill accident

To develop a comprehensive understanding of molten salt behavior during a spill, the study constructed a scenario inspired by the research of Chun et al. (2024) [2]. This study assumed a pipe breakage, causing high temperature molten salt to pour onto stainless steel in air environment, simulating the accident conditions. Moreover, the KCl-UCl3 was used in this simulation, which is widely considered as a key candidate for MSR [3].

2.2. Geometry and mesh

Figure 2 illustrate the used geometry in this study. The length and height were set as 500 mm and 150 mm for the two-dimensional geometry. The inlet was 5 mm wide and located 10 mm height, with the top and right sides simulated as outlet. The region where the molten salt flows the bottom to the inlet was divided into 510 elements horizontally and 20 elements vertically. The remaining area was meshed with 500 elements horizontally and 80 elements vertically, resulting in a total of 50,200 mesh cells.

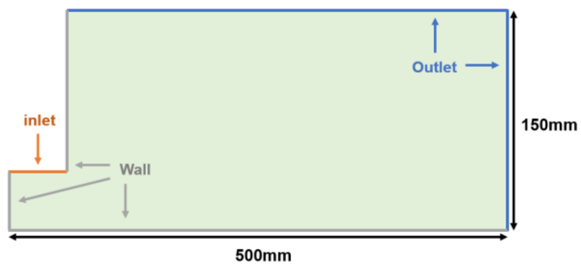

Fig. 2. A schematic of the simulated geometry for a molten salt spill accident

2.3. Development of numerical solver

In this study, it is needed to calculate the multi-phase such as liquid, solid and gas with heat transfer. To calculate the whole process, OpenFOAMv2312, an open-source CFD library, was utilized to develop a numerical solver. For the salt spill simulation some modification was conducted based on 'twoPhaseEulerFoam' solver, which is used to model multiphase flow, treating both phases as interpenetrating continua. Generally, the solver only calculates the separate phase without phase change and heat transfer without radiation. Thus, some modeling and source code development was conducted.

2.3.1 Radiation Modeling

Typically, in the case of high temperature molten salt, the radiation heat transfer is considered. Thus, the existing OpenFOAM radiation models were extended to multiphase flow to accurately simulate molten salt spill accidents. To simplify the simulation, the radiation source term Sh , which accounts for the higher temperature of the molten salt compared to air, was applied only to the molten salt phase. This source term was incorporated into the energy equation for the molten salt within the 'twoPhaseEulerFoam' solver, as defined in Eq. (1) [4]. In Eq. (1), Ru and Rp are components of the radiation source term, where Ru represents a constant component, and Rp depends on the fourth power of the absolute temperature. The values of Ru and Rp are determined by the selected radiation model, such as the P1 or fvDOM model.

$$Sh = Ru - RpT^4 \qquad (1)$$

2.3.2 Solidification Modeling

To model the solidification, modifications of the material properties were applied when the salt approached its solidification temperature. The material property values determined using linear interpolation.

Table 1 presents the properties of KCl-UCl3 at specific temperatures [5-7].

Table 1. Material properties of KCl-UCl3

Properties	573.15 K	830.15 K	831.15 K	1473.15 K
Density (kg/m^3)	4541.9	4541.9	4129.0	3347.6
Viscosity (Pa·s)	10 (for solid)	10 (for solid)	0.0023	0.0011

Properties	723.15 K	848.15 K	973.15 K
Specific heat (J/kg·K)	657.22		
Thermal conductivity (W/m·K)	0.3075	0.3005	0.2935

2.5. Parameters of OpenFOAM simulation

In this section, the overall calculation condition was provided. The turbulence model was set to laminar due to the low Reynolds number (Re) of the flow. The calculated Reynolds number is 25,909, which is well below threshold and confirms the suitability of using a laminar turbulence model. For the radiation component, the fvDOM model was used to compute radiative heat transfer. The key parameters used in the analysis are summarized in Table 2.

Table 2. Major parameters for OpenFOAM Calculation

Parameters	**Values**
Simulation	
Solver	twoPhaseEulerRadiationFoam
Turbulence model	laminar
Time step	0.001
Iteration and Discretization	
Iteration solver	PIMPLE (Pressure-Velocity coupling algorithm)
Smoother	symGaussSeidel
Time term	Euler
Gradient term	Gauss linear
Interpolation	Linear
Radiation Model	
Model	fvDOM

The initial and boundary conditions in this study were derived from the referenced research. The salt was injected at 923.15 K. The velocity of injected salt was 0.0258 m/s over a period of 100 seconds. The molten salt was discharged into air, which was modeled as an ideal gas at 298.15 K. The lower wall was set to a fixed temperature of 298.15 K to promote heat conduction, while the left wall was assigned a 'zeroGradient' to simulate the open-air space. The outlet employed a 'fluxCorrectedVelocity' condition, an OpenFOAM boundary condition used for patches with specified pressure. It applies a 'zeroGradient' to the outflow velocity initially and then corrects the velocity based on the flux to ensure accurate flow behavior.

Additionally, the radiation properties were set as follows: the emissivity of the wall was set to 1, and the absorptivity of the fluid was set to 1. A summary of the boundary conditions used in the simulation is provided in Table 3.

Table 3. Boundary conditions

Boundary conditions	Values
Temperature boundary conditions	
Inlet Outlet Bottom wall Left wall	Fixed value (923.15 K) inletOutlet (298.15 K) Fixed value (298.15 K) Zero gradient (adiabatic)
Velocity boundary conditions	
Inlet Outlet Bottom wall Left wall	Fixed value (0.0258 m/s) fluxCorrectedVelocity No slip condition No slip condition
Radiation boundary conditions	
Inlet Outlet Bottom wall Left wall	Emissivity = 1
Molten salt	Absorptivity = 1

3. Results and Discussion

To evaluate the importance of radiation heat transfer, the results were analyzed by using average temperature of salt, length of leading edge and ratio of solidification ratio. Figure 3 and 4 present average temperature of salt and solidification ratio. Regardless of radiation model applied, average temperature of salt and solidification ratio were similar at 50 seconds. After 50 seconds, average temperature of salt was lower when radiation model was applied, because of radiative heat flux. Beyond 85 seconds, the temperature of salt reached to 770 K. Between 20 seconds and 40 seconds, the temperature increase can be attributed to the reduction in conduction effects as solidification progresses at the bottom surface.

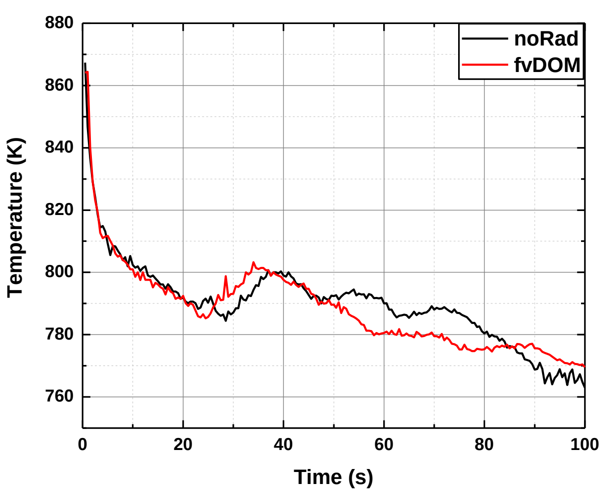

Fig. 3. Average temperature of salt based on the application of the radiation model

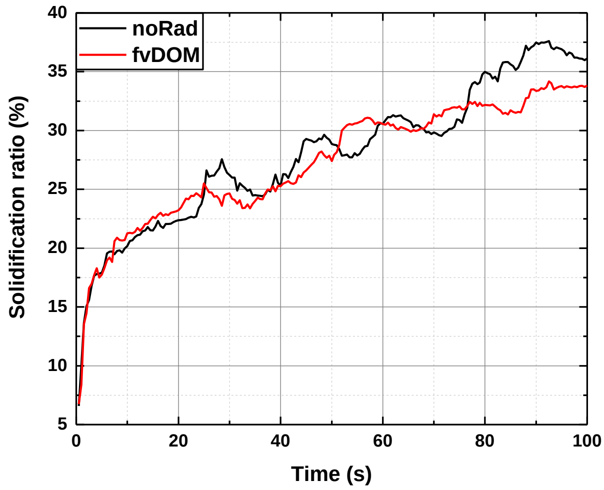

Fig. 4. Solidification ratio based on the application of the radiation model

Referring to Figure 4, there was no clear difference of solidification ratio whether the radiation model was applied. However, after 75 seconds, solidification ratio was higher when radiation model was not applied. This difference was due to the thickness of the spilled salt and the length of the leading edge. Figure 5 shows the shape of leading edge with and without radiation model at 100 seconds. In case (a), leading edge was thinner and longer than in case (b) because the application of fvDOM model led to faster surface solidification, which resulted in increased thickness. Consequently, this effect made it more difficult for the spilled molten salt to overcome the increased thickness, leading to a shorter leading edge. When the radiation model was not applied, the leading edge was longer, which resulted in more conduction. This increased conduction led to a higher ratio of solidified salt. Thus, the absence of the radiation model predicted a higher solidification ratio due to the greater length of the leading edge and increased conduction.

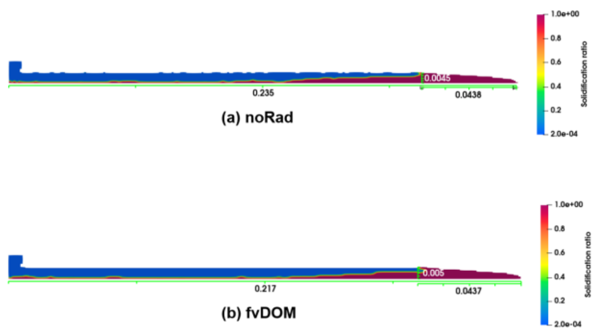

Fig. 5. Leading edge of the spilled salt based on the application of the radiation model at 100s

However, an analysis of the results shows that various parameters do not exhibit significant differences depending on whether the radiation model was applied.

Therefore, the radiative heat flux was measured to determine the impact of radiative heat transfer, and the results are presented in Figure 6. The relatively small effect of radiative heat transfer compared to conduction and convection in high temperature salts is further supported by the fact that the lower wall is fixed at 298.15 K. Boundary condition of lower wall leads to a dominant role of conduction in the overall heat transfer dynamics, thereby limiting the influence of radiation in this scenario.

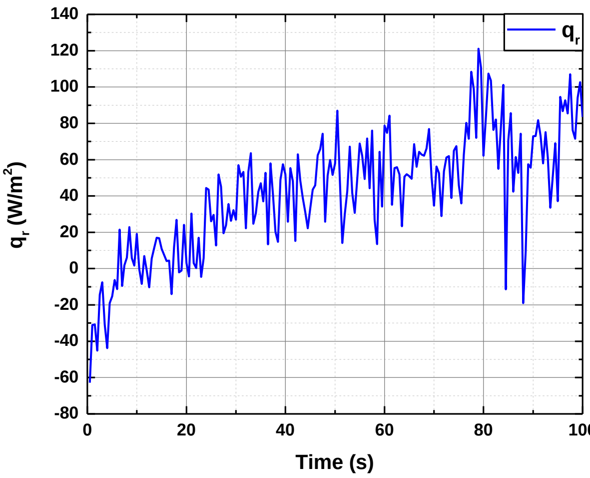

Fig. 6. Radiative heat flux in salt spill simulation

4. Conclusion

This study focused on the numerical analysis of molten salt behavior during a spill accident using OpenFOAM. The study involved modeling complex phenomena by developing the 'twoPhaseEulerRadiation Foam' solver, which extends the existing multiphase flow solver to include radiation modeling. Key findings include:

- ✓ The application of the radiation model in OpenFOAM resulted in temperature differences after 20 seconds. Beyond 50 seconds, the average temperature salt was lower when radiation model was applied.
- ✓ The length of the leading edge was shorter when the radiation model was applied in OpenFOAM due to thickness of spilled salt.
- ✓ The percentage of solidified salt relative to the total salt volume did not show a significant difference whether the radiation model was used in OpenFOAM.
- ✓ Analysis of molten salt spill accident using OpenFOAM with the radiation model indicates that radiative heat flux was not a significant parameter affecting the results of this study.

This study analyzed high temperature molten salt leakage within a multiphase flow scenario with radiation modeling. Future research should aim to enhance the solver by improving the accuracy of radiative heat transfer assessments. The goal is to ensure that radiative heat transfer, alongside conduction and convection, has a substantial impact on the overall heat transfer mechanisms.

Acknowledgements

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