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Preliminary CFD Analysis of Spreading and Solidification of FLiNaK and KCl-UCl_3

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1. Introduction

Molten Salt Reactors (MSRs) are highly anticipated to exclude severe accidents such as meltdowns in pressurized water reactors [1-3]. However, to confirm the safety of molten salt reactors, the behavior of the molten salt leaked under anticipated condition needs to be investigated thoroughly. The molten salt is easily solidified even if leaked, and most radioactive materials including fission products are expected to be captured inside in the molten salt. Nonetheless, the technical basis at present is insufficient and needs to be verified [4,5].

Since the thermal property information on leaked molten salt and fission products is not abundant, it is necessary to secure technical criteria based on preliminary experiments or numerical simulations. If any relevant preliminary analyses indicate that the cooling of the molten salt is insufficient, it is necessary to secure safety component such as catchers to the containment vessel to cool the leaking molten salt. In other words, it is necessary to evaluate and verify if the integrity of the containment vessel can be maintained, and if radioactive material does not leak into the nuclear systems with the introduction of the catcher. Minimizing the radioactive material release during a hypothesized accident is essential not only to satisfy regulatory requirements but also to protect the public and environment [6,7]. Figure 1 shows a schematic of possible physical phenomena in the event of a molten salt leak [8].

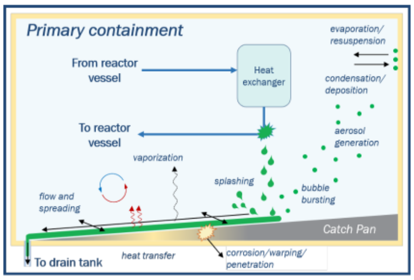

Fig. 1. A schematic of molten salt leaking from the MSR and spilling onto the catcher.

In 2022 Argonne National Laboratories (ANL) utilized MELTSPREAD code to simulate spread behavior of a molten salt reactor. An accident was assumed that 5 L of molten salt (FLiNaK-based) leaked to the bottom through a 1/4-inch rupture at 12 L/hr. The behavior of the molten salt was analyzed according to the initial temperature, initial decay heat, and leakage flow rate. As a result, it was confirmed that the temperature of the molten salt increased due to insufficient heat transfer to the outside when the decay heat of the molten salt was considered. Thus it was concluded that a separate facility capable of cooling the leaking molten salt would be necessary in the event of a molten salt leakage accident [9].

However, MELTSPREAD code was developed with optimization of the corium spread from the pressurized water reactor. So the molten salt obviously different with the corium may not be simulated accurately by the MELTSPREAD. However, there exist very few experimental and numerical results regarding the molten salt. Thus this study tried to compare the behavior of FLiNaK and KCl-UCl_3 by using the ANSYS Fluent code.

2. Numerical method and condition

2.1. Geometry and mesh

ANSYS Workbench is a pre- to post-processing platform for numerical simulation. Figure 2 shows a schematic of the analysis domain for leaking molten salt. To calculate the leakage of 5,000 cc of molten salt into a flat catcher, a 2D axisymmetric domain with a radius of 500 mm and a height of 100 mm was created. The inlet is set to near the floor to exclude the effects of jet collisions. We also defined the top and sides as outlets. The inlet is a 5mm radius as in ANL/CFCT-22/15. The catcher is made of 6.35mm thick stainless steel 304 and the bottom boundary of the catcher is insulated.

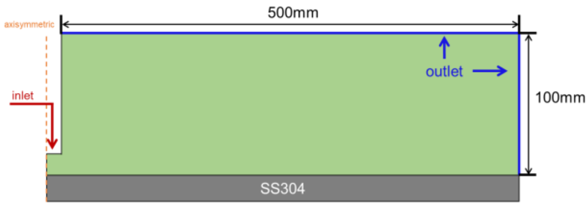

Fig. 2. Domain of leaking molten salt numerical simulation.

To improve the stability of the convergence, y+ is targeted at 12 or higher, and the meshing utilizes ICEM CFD to generate 13,790 rectangular meshes. The mesh size near the inlet is 1.25 mm radial and 1.25 mm high. Mesh sensitivity tests were performed using four different meshes, ranging from approximately 8,000 to 16,500.

2.2. Analysis code

The numerical simulation of molten salt leaking was performed using ANSYS Fluent 2022R1, the most popular numerical simulation tool. Realizable k-epsilon was used for its convergence stability. The VOF model is used to calculate the heat transfer interaction of air-molten salt. The DO model is used to calculate the radiative heat transfer of molten salt at high temperatures. The solidification and Melting model is used to calculate the solidification of molten salt when it is exposed to room temperature and cools down. Table 1 shows the models used in this simulation.

Table. 1. Fluent Settings

Setting	Fluent	
Multiphase	VOF	-
	Volume Fraction Parameters	Implicit
	Surface tension	-
Turbulent model	Realizable k-epsilon	-
Radiation model	Discrete Ordinates	-
Solidification	Mushy zone parameter	1e+5
	Pull Velocities	Included
Scheme	PISO	Bounded second order implicit
Time step	0.005s	30 iter/time step
Calculation time	Simulation time: 25min	Intel 13900K(20core): 1 week

2.3. Boundary conditions

FLiNaK, used in ANL/CFCT-22/15, and KCl-UCl_3, is a strong candidate for molten salt that could be used in MSRs [9,12,13]. As initial conditions, the space into which the molten salt is poured is filled with ideal-gas-air at 300 K, with air entering and leaving through an outlet. The molten salt is leaked at a volumetric flow rate of 12,000 cc/hr, which is converted to a velocity-inlet condition of about 0.04 m/s, 923 K, and set to leak for 25 min. The catcher is made of stainless steel 304, which has high resistance to molten salt corrosion, and the bottom of the catcher is insulated according to ANL/CFCT-22/15. These boundary conditions are summarized in Table 2. The physical properties of FLiNaK and KCl-UCl_3 are summarized in Table 3.

Table. 2. Boundary conditions

Boundary condition	Value
Pour temperature	923K
Pour volume	5000 cc
Inlet velocity	0.04m/s during 1,500 s
Substrate material	Stainless steel 304
Radius of pour jet	5 mm
Substrate thickness	6.35mm
Decay heat	None
Atmosphere	Ideal-gas-air,1 atm, 300K

Table. 3. Molten salts Properties

Properties @923K	FLiNaK	KCl-UCl_3
Density (kg/m^3)	2020	3685
Specific heat (J/kgK)	1952	657
Thermal conductivity (W/mK)	0.85	0.2963
Viscosity(cP)	3.18	1.8
Latent heat (J/kg)	399,000	70,000
Surface tension (N/m)	0.179	0.1287

3. Results and discussions

3.1. Compare with MELTSPREAD and Fluent

Figure 3 shows the leading edge plotted over time for the MELTSPREAD code and Fluent code for ANL/CFCT-22/15 using FLiNaK for 100 seconds. MELTSPREAD shows a slowly developing leading edge until 40 seconds and then predicts that the leading edge stops at about 9.5 cm after 40 seconds. Fluent showed an irregular leading edge up to 30 seconds, followed by a linear leading edge after 30 seconds, and a continuing to increase trend after 100 seconds.
In the Fluent base case, the leading edge of the molten salt appeared to move backward, which was due to the molten salt at the leading edge falling away from the main pool, reducing the leading edge of the main pool.

40 seconds after the leaking, we predicted that the molten salt in MELTSPREAD no longer spreads in a radial direction, but in a height direction. This is because the molten salt leading edge of MELTSPREAD was predicted to solidify and create a barrier to additional spreading. Moreover, limitations of MELTSPREAD include (1) the unable to simulate natural convection within the molten salt and at the molten salt-air contact, and (2) the inability to form solidification at the molten salt-catcher interface. These are factors that increase the uncertainty in the spreading behavior of MELTSPREAD.

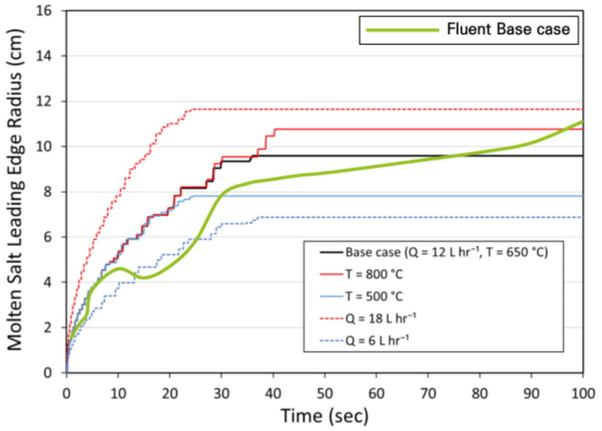

Fig. 3. The spreading of FLiNaK on flat SS304 compare with MELTSPREAD and Fluent.

3.2. Compare with FLiNaK and KCl-UCl₃

Figure 4 shows the behavior of FLiNaK and KCl-UCl_3 during 1500 s using the Fluent code. For FLiNaK, the behavior was irregular until 600 s and then exponentiation after 600 s. For KCl-UCl3, there was exponential growth from immediately after the eruption to the end of the eruption. The reason for the different characteristics of the two graphs seems to be due to the difference in physical properties such as surface tension and latent heat of the two molten salts.

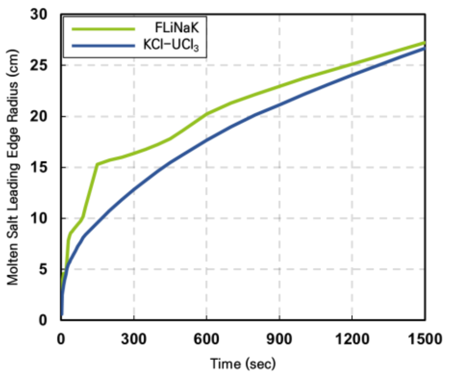

Fig. 4. The spreading of FLiNaK and KCl-UCl_3 on flat SS304 with Fluent.

Figure 5 shows the behavior of FLiNaK and KCl-UCl3 at 100, 300, and 1400 seconds. The blue part is the air region, and the red part is the molten salt region. Both molten salts spread over time with similar trends in leading-edge development. The horizontal axis shows the spreading radius of the molten salt, and the vertical axis shows the height of the molten salt. At all the time points, the leading-edge shape was predicted to be more rounded for FLiNaK, which is likely due to the higher surface tension of FLiNaK.

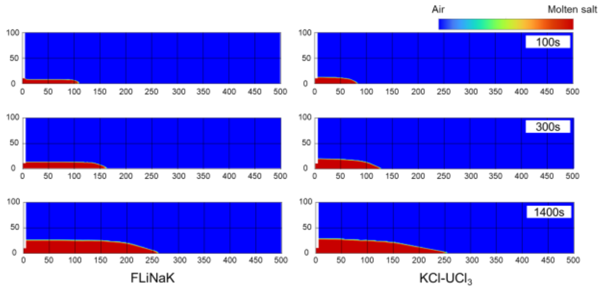

Fig. 5. The spreading behavior of FLiNaK and KCl-UCl3 on flat SS304 at 100s, 300s, and 1400s.

Figure 6 shows the solidification of the molten salt. For both molten salts, solidification proceeded from the leading edge. The leading edge of the molten salt is the center, and the liquid molten salt in the center rides over the leading edge. KCl-UCl_3 solidified faster due to its smaller specific heat and phase change heat. It was predicted that the solidification of the ejected molten salt proceeded from the top to the bottom first due to heat transfer to the substrate and heat transfer to the atmosphere.

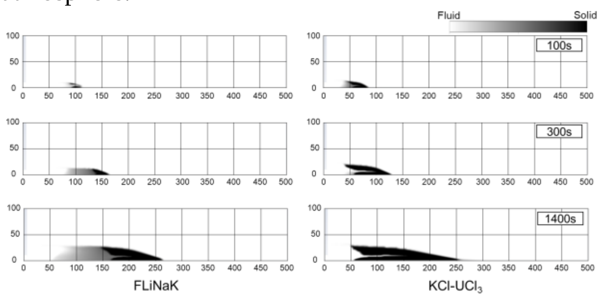

Fig. 6. The Solidification of FLiNaK and KCl-UCl_3 on flat SS304 at 100s, 300s, 1400s.

4. Conclusions

In this study, FLiNaK was used to compare MELTSPREAD and Fluent codes, and KCl-UCl_3 and FLiNaK were compared with Fluent. The spreading radius, spreading behavior of the molten salts, and solidification progress were obtained. Both leaked molten salts showed great solidification progress, confirming the inherent stability of the molten salt. The main results are presented in the following paragraphs.

- MELTSPREAD code showed a spread radius of about 10 cm, while Fluent showed about 27 cm. MELTSPREAD underpredicted the spreading radius of the molten salt. This is because MELTSPREAD was developed to calculate Pressurized Water Reactor corium and is still under development and there are physics that are not included. In the future, the model will be improved to include crust formation at the molten salt-catcher boundary and natural convection inside the molten salt.

- FLiNaK and KCl-UCl_3 differed in the fast-spreading development rate, with most properties differing by more than a factor of two, but after a long time, the spreading behavior was almost very similar. This should be analyzed through property sensitivity evaluation.
- The leaking molten salt started solidification from the leading edge first and gradually developed solidification toward the center. It was observed that solidification occurred first at the top and bottom of the molten salt due to heat transfer with the atmosphere and the catcher.

Therefore, a property value sensitivity assessment of the leaking molten salt can provide important considerations for the design of future catchers. Research on the design of improved catchers for faster solidification of leaking molten salt should be continued.

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