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Numerical Study on Relocation Process of Al, Fe, and Pb by Using the Moving Particle Semi-Implicit Method During Severe Accident of Reactor

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Abstract. Reactor safety is one of the essential parts of reactor research, especially to appropriately respond when melts down occurred during a severe accident. In this study, the relocation process of Al, Fe, and Pb was simulated by using the Moving Particle Semi-Implicit method to study the relocation mechanism of the liquids when they experienced an interaction between liquids at high temperatures. It is obtained that, to reach the stratified condition, Pb-Al needs 0.63 seconds, Al-Fe and Al-Pb need 1.14 seconds, and Fe-Al needs more than three seconds. Overall, the results indicate that the difference in viscosity and density between two liquids influences the time to reach the stratified condition. The greater the density difference between two liquids, the faster the stratification process.

Keywords: Liquid flow; Moving particle semi-implicit; Relocation process; Severe accident of a reactor

1. Introduction

Reactor safety is one of the substantial matters that should be concerned in the study of the reactor. The reactor accidents of Three Miles Island, Chernobyl, and Fukushima have warned nuclear researchers to care about the importance of reactor safety. Information about the behavior of some reactor materials (Talaat *et al*., 2019; Chandran *et al*., 2018) is very urgent to be provided. The relocation of melting material during a severe accident is an important phenomenon due to its influence on the heat transfer to the lower plenum of the reactor, which may affect the breaching of the reactor.

Several studies have been conducted regarding the relocation of molten corium. Moreover, stratification during the accident is also important to be understood to predict the failure of the reactor pressure vessel (Li *et al*., 2013). During a severe accident, the variation of materials may lead to several combinations of interaction between two materials. In the research reactor, Fe-Al interaction may need to be understood since Al is the main material with parts of Fe (Hainoun, Ghazi, and Alhabit, 2019; Farrell, 2012). On the other hand, in the LFR (Lead-cooled Fast Reactor), a study of Pb-Fe interaction in the liquid phase is needed. The reason is that Pb is the main coolant and Fe is the main structural material (Mustari and Takahashi, 2011; Machut *et al*., 2007), where Al is proposed as the outer layer of structural material (Knebel *et al*., 2000) in the Accelerator

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Driven System (ADS). Unfortunately, investigations on these material combinations in the liquid phase are very limited.

Some experiments about reactor core accidents are complicated or costly to be performed. Although experiments are still principal for some cases, computational simulations (Aliffrananda *et al*., 2022; Utama *et al*., 2021) can be an alternative to reduce the complexity or the cost of experiments. On the other hand, the conventional mesh methods face difficulty in explaining several melted core phenomena, i.e. stratification case, free-surface flow, and phase transitions. The Moving Particle Semi-Implicit (MPS) method introduced first by Koshizuka and Oka (1996) is one of the alternative mesh-free methods utilized to simulate the relocation process of some nuclear materials. This method has been applied successfully (Duan, Yamaji, and Sakai, 2022; Masumura, Yamaji, and Furuya 2015; Mustari *et al*., 2015; Li, Oka, and Furuya, 2014; Kawahara and Oka, 2012) as reviewed by Li *et al*. (2020).

While there are many studies analyzing melting interactions between the melted core and solid materials during reactor core melting, there is still limited simulation on the relocation of molten fluids. Studies of the relocation process of some liquids were performed by some researchers, such as Li *et al*. (2013) with silicon oil and salt water, Ilham *et al*. (2018) with freshwater, and Hidayati *et al*. (2021) with cooking oil and freshwater. In this study, the liquids of Al, Fe, and Pb are utilized. The simulation of the relocation process is one of the visible solutions for understanding the phenomena in the reactor accident. Therefore, the study of the relocation process is utterly substantial to be performed for nuclear materials. Due to the lack of study on the materials in the case of a severe accident, where most materials are in the liquid phase, the objective of this study is to simulate the relocation process of some liquids of nuclear materials (Al, Fe, and Pb) and the contact process between two liquids with various temperatures.

2. Methods

2.1. Mathematical Model and Numerical Method

The Moving Particle Semi-Implicit method assumes that a particle only exercises an interaction with a limited number of its nearest particles as shown in Figure 1. To accommodating this assumption, the weight function exists as described well in the paper of Koshizuka and Oka (1996), including the explanation of the particle number density, the gradient, the divergence, and the Laplacian models. All equations in the MPS method follow the mass and the momentum conservation equations as the commonly used governing equations for incompressible flow where (Koshizuka and Oka, 1996).

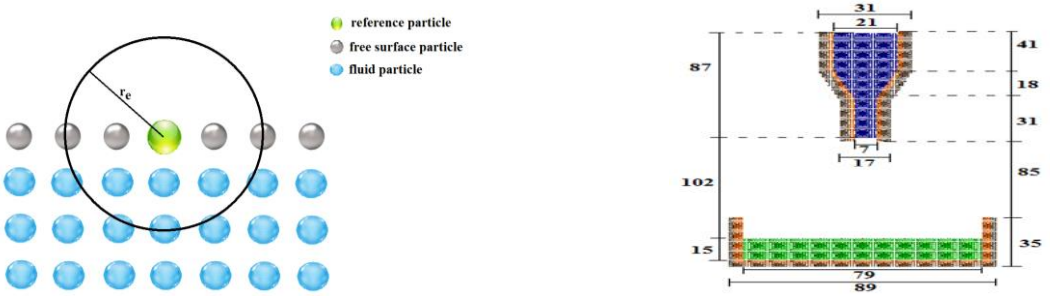
$$\frac{D\rho}{Dt} = \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) = 0 \tag{1}$$

$$\frac{D\vec{u}}{Dt} = \vec{g} - \frac{1}{\rho}\nabla P + \nu \nabla^2 \vec{u} \tag{2}$$

In the equations above, the density is represented by ρ, the time is represented by t, the velocity vector is represented by $\vec{u}$, the gradient is represented by ∇, the gravity is represented by $\vec{g}$, the pressure is represented by P, and the kinematic viscosity is represented by ν. To assist the calculation process, the numerical calculations are proceeded explicitly by using the finite difference method and implicitly by using the Crank-Nicholson method (Koshizuka and Oka, 1996). Here are the references that explained the MPS method clearly, including the algorithm (Li *et al*., 2020; Kawahara and Oka, 2012; Koshizuka and Oka, 1996).

2.2. Simulation

In this study, two types of liquids were used, namely, the fallen liquid placed inside the 2D containment and the target liquid placed inside a bottle located 102 mm above the surface of the target liquid. Both liquids are chemically miscible, and it was assumed that the stratification process in thermal-hydraulic is faster than in the chemical process, as supported by references (Mustari *et al*., 2015; Mustari and Oka, 2014), these liquids can be considered as an immiscible liquid. The temperature, density, and kinematic viscosity of each used liquid can be seen in Table 1. The simulation was performed by using 4139 particles and a similar code of these references (Yulianto *et al*., 2019; Ilham *et al*., 2018).



(a) Free surface boundary condition (b) Initial condition (in mm)

Figure 1 Boundary (a) and initial (b) condition (in mm)

Table 1 The parameters of each liquid (IAEA, 2008)

Component	$T_{melting}$ (°C)	$T_{boiling}$ (°C)	$T_{simulation}$ (°C)	Density (kg m^{-3})	Kinematic viscosity (m^2 s^{-1})
Al	660	2,519	1,600	2.084890×10^3	7.382931×10^{-4}
			1,800	2.022690×10^3	7.083604×10^{-4}
			2,000	1.960490×10^3	6.846094×10^{-4}
Fe	1,538	2,861	1,600	6.977548×10^3	2.050208×10^{-3}
			1,800	5.115362×10^3	1.784475×10^{-3}
			2,000	4.930162×10^3	1.591594×10^{-3}
Al	660	2,519	1,200	2.209290×10^3	8.295089×10^{-4}
			1,400	2.147090×10^3	7.771429×10^{-4}
			1,600	2.084890×10^3	7.382931×10^{-4}
Pb	327	1,745	1,200	9.590534×10^3	8.123931×10^{-8}
			1,400	9.342134×10^3	6.835953×10^{-8}
			1,600	9.093734×10^3	5.823038×10^{-8}

3. Results and Discussion

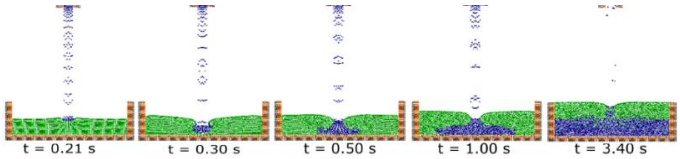
3.1. The Relocation Profiles

The relocation process of Fe-Al can be seen in Figure 2 where all temperatures have a similar pattern, where Fe made a contact with Al, broke through the Al layer, dived, created a layer under the Al layer, and reached the stratified condition. When colliding with the target liquid, Fe could break through Al as presumed that Fe has a greater density than Al. The relocation process of Al-Fe can be seen in Figure 3 where all temperatures have a similarity in its pattern where Al made a contact with Fe, floated above the Fe layer, made a layer in that position, and finally reached the stratified condition. When colliding with the target liquids, Al cannot equalize the buoyancies of Fe. It forces Al to move on top of Fe and create a layer above that liquid. It is because Al has a lower density than Fe. It is presumed that the liquid with greater density needs more effort to break the layer of the target liquid and dives under that layer. In the stratification process, the lower density moves down gradually to form a layer under the higher density. The higher viscous force that dominates

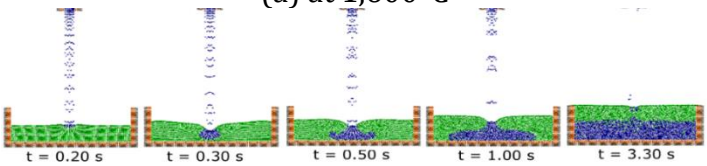
the stratification process is expected as the reason for this phenomenon. The collision time and the time to reach the stratified condition for all used temperatures are similar. The collision time was reached in 0.16 seconds and the stratified condition was reached in 1.30 seconds.

The relocation process of Al-Fe can be seen in Figure 4. The relocation process in this case has a similar pattern to the relocation process of Al-Fe. The time collision and the time to reach the stratified condition are similar to those of Al-Fe, except for the collision time at 1,400°C where Al-Pb reached it in 0.17 seconds. The relocation process of Al-Fe can be seen in Figure 5 where Pb collided with Al in 0.13 seconds and made splashes that reached up to the height of the containment. These splashes were gone out at 0.37 seconds. After that, Pb formed gradually a layer below Al and commenced the stratification process at 0.37 seconds. The stratified condition of Pb-Al is achieved at about a second for all temperatures. These obtained results are similar to the cases of Pb-Al although the temperature was different.

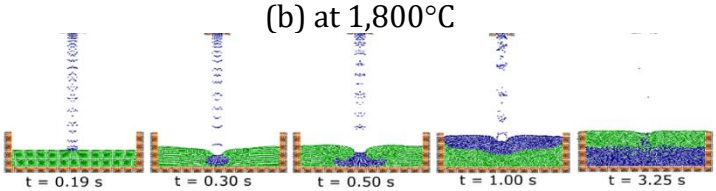
From those results above, compared to Al and Fe, Pb left the bottle and reached the surface of the target liquid in the fastest time among the used combinations. It results because, still as the presumption, the density of Pb is the greatest among them. Besides, the kinematic viscosity of Pb is the smallest among them. It makes Pb flow out of the bottle container easily. However, it still needs further study for verification. Next, the focus is targeted at the collision between liquids. In this study, the relocation process without splashes has been found in the cases of Fe-Al, Al-Fe, and Al-Pb. The relocation process with splashes has been found in the Pb-Al. When Pb-Al was run, the splashes were obtained. When switching to Al-Pb, the splashes were not obtained. It means that the splash will arise if the fallen liquid has a higher density when the difference in density between the two is great enough. The time duration was counted as follows. The timing of collision started when the two liquids made direct contact. Both liquids are considered to reach the stratified state if two layers have formed along the length of the container. The summary of time, for all cases, is performed in Figure 6 where at 2,000°C, to make a contact and to reach the stratified condition, Al has the fastest time among the other temperatures.



(a) at 1,600°C

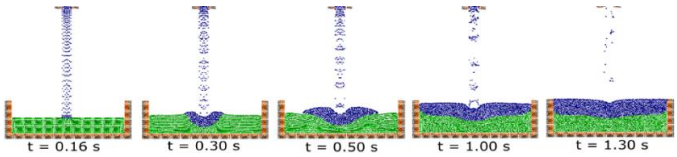


(b) at 1,800°C

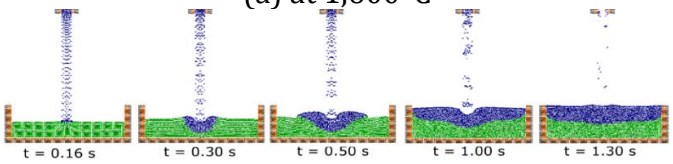


(c) at 2,000°C

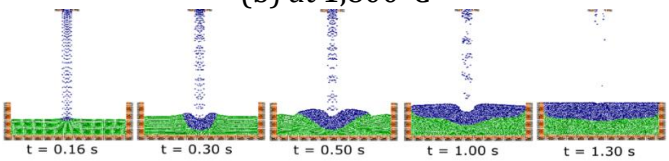
Figure 2 Relocation process of Fe–Al



(a) at 1,600°C

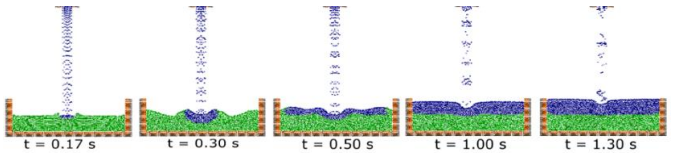


(b) at 1,800°C

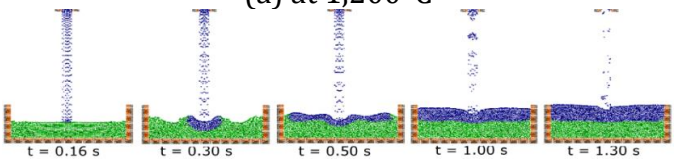


(c) at 2,000°C

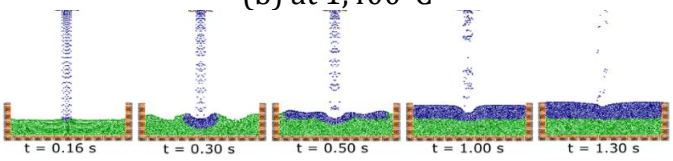
Figure 3 Relocation process of Al–Fe



(a) at 1,200°C

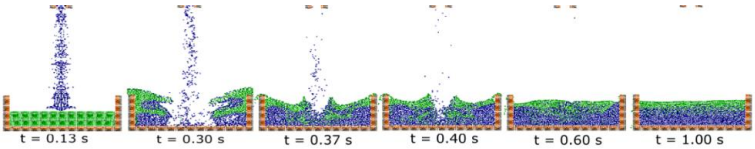


(b) at 1,400°C

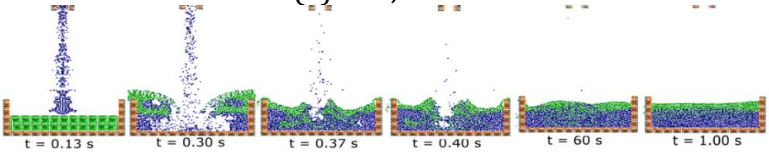


(c) at 1,800°C

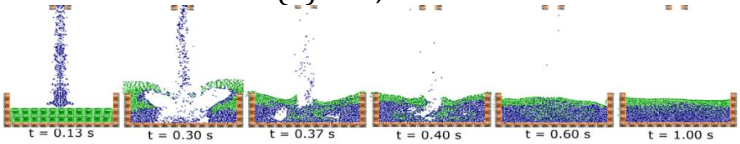
Figure 4 Relocation process of Al–Pb



(a) at 1,200°C



(b) at 1,400°C



(c) at 1,800°C

Figure 5 Relocation process of Pb–Al

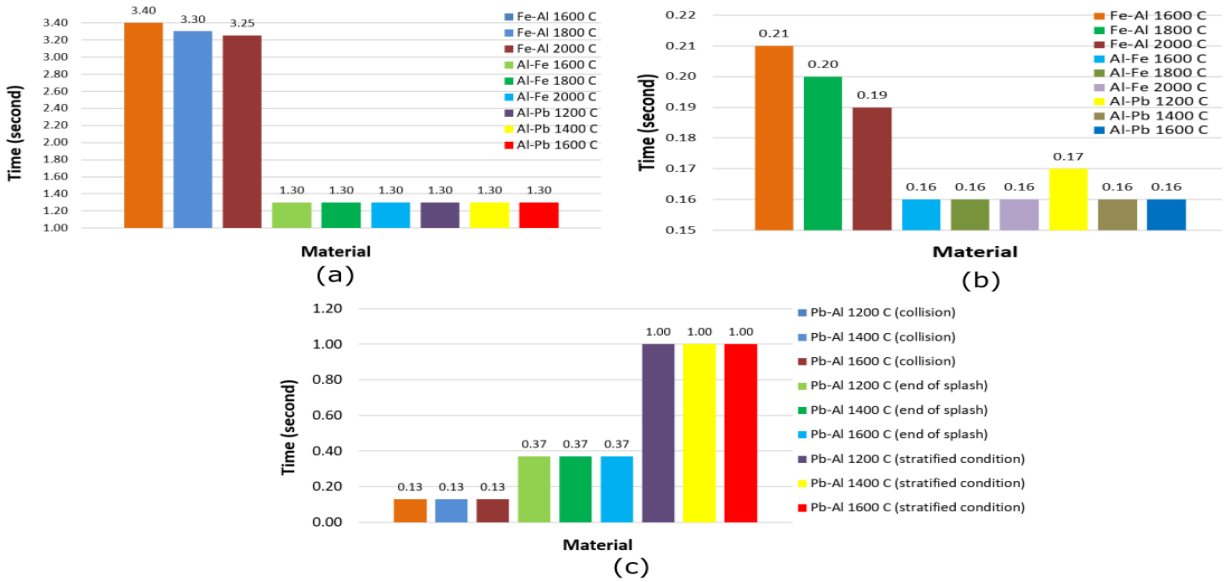


Figure 6 The time summary for the relocation process

3.2. The Pressure Profiles

The pressure profiles of Fe-Al can be seen in Figure 7. The higher pressure commenced in the middle of the container and expanded to the corner of the container. In Figure 8 part (a), the pressure profiles in two spots at the bottom of the container were investigated, i.e the left-bottom side and the center-bottom side. The center-bottom side has higher pressure than the left-bottom side. The results of Fe-Al at 1,600°C have higher pressure than the other temperatures in this case. The pressure profiles of Al-Fe can be seen in Figure 9. The patterns of these results are similar to the pattern of Fe-Al. The higher pressure is still found in the bottom of the container. The pressure profiles inside the container in Al-Fe can be seen in Figure 8 part (b). The results of Al-Fe at 1,600°C have the highest pressure among the results in this case as found in Fe-Al.

The pressure profiles of Pb-Al can be seen in Figure 10. In that figure, it can be seen that the pressure profiles are similar to those of Fe-Al and Al-Fe. The bottom side of the container has higher pressure than the wall. The pressure profiles inside the container are displayed in Figure 8 part (c). In that figure, it can be seen that the pressure is higher between 0.2 seconds and 0.4 seconds than the others. It is the condition when the splash was arising. The splashes make the pressure high. The pressure profile of Al-Pb can be seen in Figure 11. The results of this case are similar to those of Fe-Al and Al-Fe. The pressure profiles inside the container in this case can be seen in Figure 8 part (d). The pressures are mostly in a disarray pattern. In regards to stratification, the difference in density is the driving mechanism. Therefore, a higher density difference will accelerate the stratification formation. The stratification will start from the below area of the less dense material (Yulianto *et al*., 2018; Li *et al*., 2013).

From the obtained results, the relocation pattern of the liquids is similar to the results obtained by Ilham *et al*. (2018) using a different liquid, where the MPS result is compared to the experiment. Therefore, it is expected that the temperature did not significantly impact the relocation process, which agrees with Hidayati *et al*. (2020). Furthermore, the splash pattern of this study is similar to the results of Hidayati *et al*. (2021). The splash will arise if the fallen liquid has a higher density where the difference in density between the two is big enough. The viscosity also affects the formation of the splash. High-viscosity fluid will show less splash formation than molten tin relocation (Li, Oka, and Furuya, 2014).

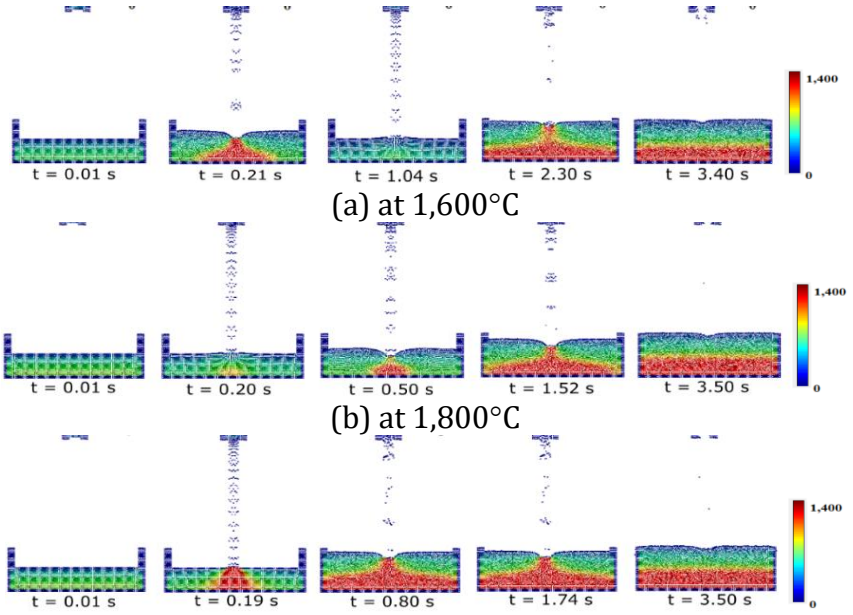


Figure 7 The pressure profiles of Fe-Al (The pressure unit is in N/m^2)

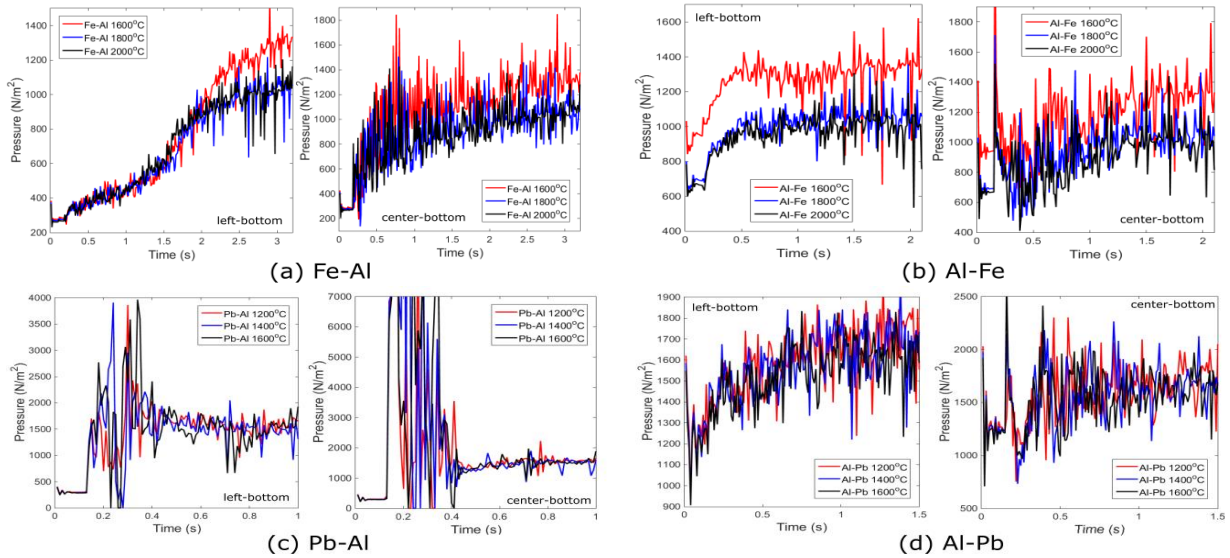
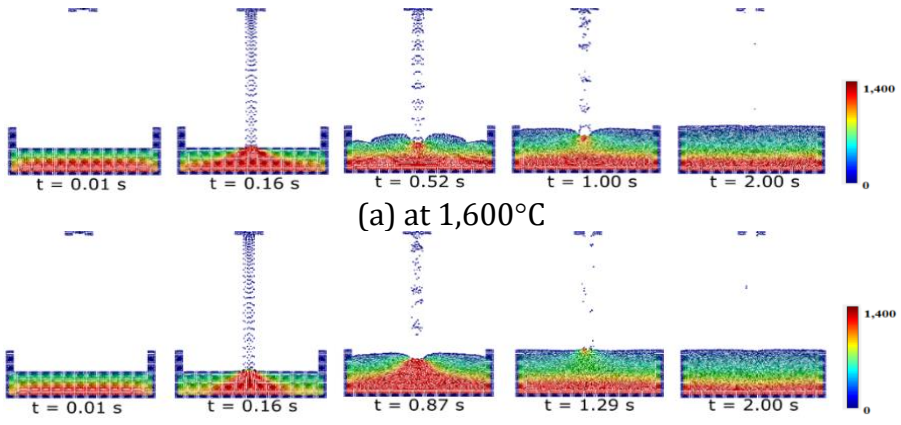
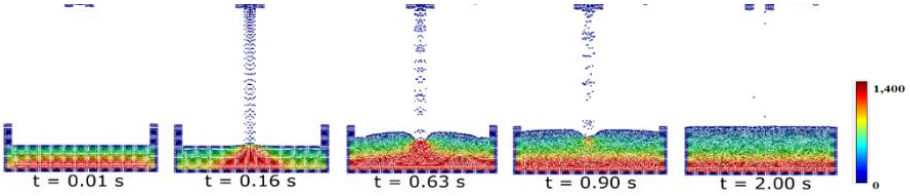


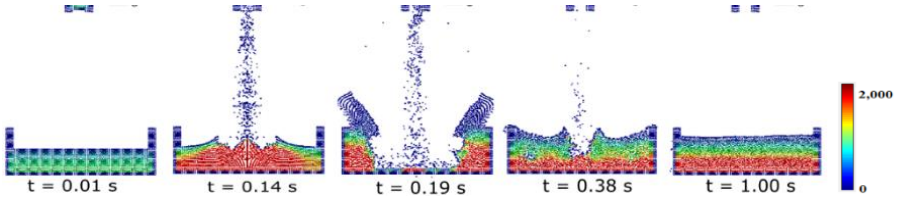
Figure 8 The pressure profiles (in N/m^2) inside the container for all configurations



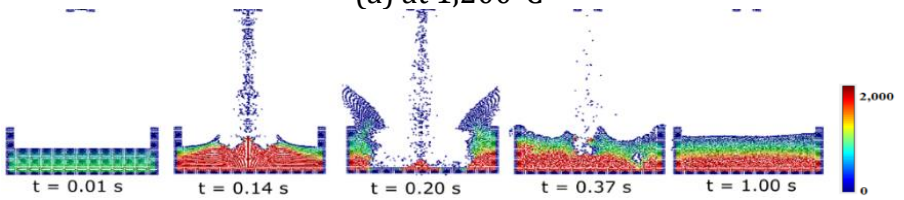


(c) at 2,000°C

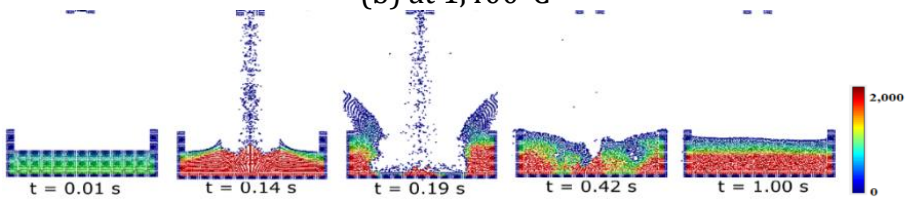
Figure 9 The pressure profiles of Al-Fe (The unit of pressure is in N/m^2)



(a) at 1,200°C

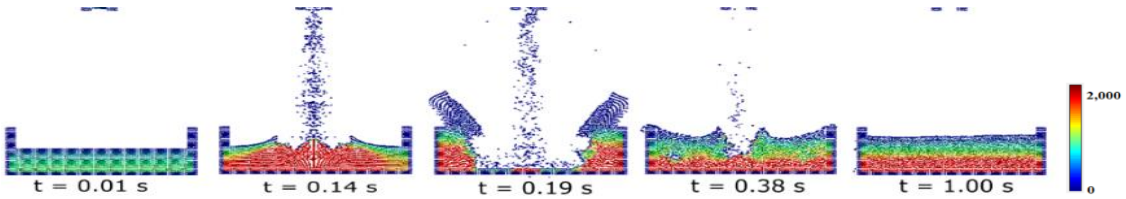


(b) at 1,400°C

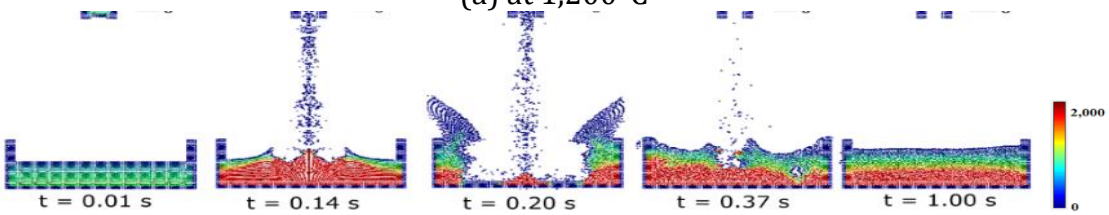


(c) at 1,600°C

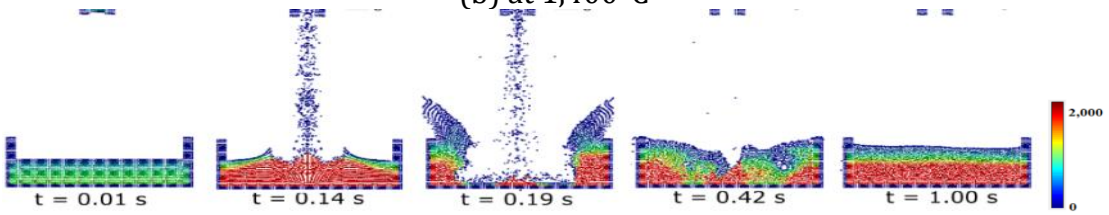
Figure 10 The pressure profiles of Pb-Al (The unit of pressure is in N/m^2)



(a) at 1,200°C



(b) at 1,400°C



(c) at 1,600°C

Figure 11 The pressure profiles of Al-Pb (The unit of pressure is in N/m^2)

Ideally, the present result should be validated by the experiment result; however, it is very difficult to find a study on Pb, Al, and Fe interactions. Regarding Pb-Al, there is an experiment of melting and solidification, however, it is for crystalline size (Grabaek and Bohr, 1965). In the case of the melting behavior of Pb-alloy with silicone oil, Masumura *et al*. (2015) successfully validated the experiment with numerical simulation.

During severe reactor accidents with several thousand degrees Celsius of temperature, the existence of the splash may significantly affect the heat transfer process and thus melting progression. In that regard, a study on the splash effect on melting progression is the area to be investigated. The results give an important understanding of how the pressure may affect the lower plenum of the reactor when the liquids are relocated. Based on the results above, the bottom side has higher pressure than the wall side. In a nuclear reactor, the pressure profiles during a severe accident can provide essential information for the prediction of the breaching and also give insight to the manufacturer of the reactor. The present results are focused on the relocation process and its splash, in the future, more realistic geometry and condition close to the reactor situation during the accident is necessary to give a better understanding of the relocation. It is also essential to compare the results with the experiment or the other methods.

4. Conclusions

The relocation process of some liquids has been investigated in this study. The MPS method has been utilized to simulate the stratification process of these liquids. This study shows that Pb-Al needs 0.13 seconds to reach collision, Al-Fe and Al-Pb need 0.16 seconds, and Fe-Al needs more than 0.19 seconds. To get the stratified condition, Pb-Al needs 0.63 seconds, Al-Fe and Al-Pb need 1.14 seconds, and Fe-Al needs more than three seconds. It is also found that the difference in viscosity and density between two liquids influences the time to reach the stratified condition — the more significant the density difference between two liquids, the faster the stratification process. The obtained results in this study are in a preliminary stage, which means that further study needs to be conducted in both experiment and simulation.

Acknowledgments

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