THE STRATIFICATION BEHAVIOR OF REACTOR MATERIALS IN THE FRAMEWORK OF MOVING PARTICLE SEMI-IMPLICIT

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Abstract *In reactor research, the safety of the reactor plays an important role. Besides the experiment research, computational simulation can also provide important information about the behavior of materials inside the reactor core. The Moving Particle Semi-Implicit (MPS) method assists in providing information about the reactor material computationally. In this study, the stratification process of several materials, i.e. the melts of PbBi, PbLi, and Pb in combination with Al, have been investigated by simulation. The time to achieve stratified conditions for each material has been obtained where each paired material needs 0.5 seconds to reach the stratified condition. It is also obtained that the Pb-Al is the fastest in reaching the stratified condition among the other used materials.*

INTRODUCTION

The safety of the reactor is one of the important things that should be concerned in reactor research. The study about the behavior of reactor materials is very essential to be performed. Conceptually, it can provide an important information about the behavior of the reactor materials in the case of reactor accident. Some experiments about reactor core accidents are difficult and costly to be performed experimentally. The conventional simulation methods, i.e., independent of empirical correlations, have also difficult to analyze several melted core phenomena, such as stratification, free-surface flow, and phase transitions. Understanding the behavior of the materials when interacting with the other materials is a valuable information during reactor accident, like the Fukushima accident, where the reactor core was melted. Knowing this information is a fundamental reference to perform an accurate counter measurement.

The computational simulation can provide an alternative way to solve those problems. Reducing the cost of experiments is one of the advantages of computational simulation. To simulate the melted core phenomena, especially to analyze the incompressible free surface flow, it can be utilized the meshless particles method so-called Moving Particle Semi-Implicit (MPS) method. Koshizuka and Oka were the researchers who first introduce this method (1). This method has been applied in nuclear engineering research (2–6) as reviewed by Gen Li et al (7).

The stratification behavior of some materials that have been investigated are tin-NeoSK-SALT (6), silicone oil-salt water (8), and cooking oil-lubricant oil-fresh water (9). In this study, the stratification process of some nuclear materials, such as PbBi, PbLi, Pb, and Al, has been performed to provide preliminary information. It is a piece of valuable information in nuclear reactor research, especially for the case when the reactor core melts down. The liquids of PbBi and Pb are used as a coolant in some conceptual designs of fast reactors (10–11). The liquids of PbBi and PbLi are used as blanket material in fusion reactor (12–13). Aluminum is applied to manufacture the claddings of uranium units in reactors and the structural materials in research reactors.

In this study, these materials (PbBi, PbLi, Pb, and Al) have been investigated to understand its behavior in the stratification process by using the MPS method. The algorithm and the source code have been adopted from the study about

the stratification behavior of immiscible liquids (9). The stratification process of these materials is simulated to obtain preliminary information about the process of some reactors.

METHODS

It is commenced with the continuity equation (law of mass conservation) and the Navier-Stokes equation (law of momentum conservation) as the commonly used governing equation for incompressible flow, which can be described as (1)

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

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

Where ρ is the density, t is the time, $\vec{u}$ is the velocity vector, ∇ is the gradient, $\vec{g}$ is the gravity, P is the pressure, and ν is the kinematic viscosity. In analyzing incompressible flow, the MPS method approaches the fluid as the meshless moving particles with constant mass. The motion of these particles constitutes convection. This condition makes the numerical diffusion, a problem for Eulerian approaches, become uncountable.

Theory

Therefore, in the MPS method, the reference particle only makes interaction with a finite number of nearest particles. The interaction force is only between the two nearest particles. By using the weight function, as a function of the distance, this interaction force can be calculated. The weight function which is commonly used in the MPS method can be explicated as

$$w(r) = \begin{cases} \left(1 - \frac{r}{r_e}\right)^2 & 0 \le r \le r_e \\ 0 & r_e \le r \end{cases} \quad (3)$$

Here, r represents the distance between two particles and re represents the finite radius for limited interaction. The approximation value of the weight function can be found in the reference (1). The weight function reaches to be zero when the distance between the two nearest particles is greater than the finite radius. The particle number density, which is proportionate to the liquid density, on the i-particle position can be written as

$$n_i = \sum_{j \ne i} w\left(|\vec{r}_j - \vec{r}_i|\right) \quad (4)$$

Where $\vec{r}_i$ and $\vec{r}_j$ are position vectors of i and j particles.

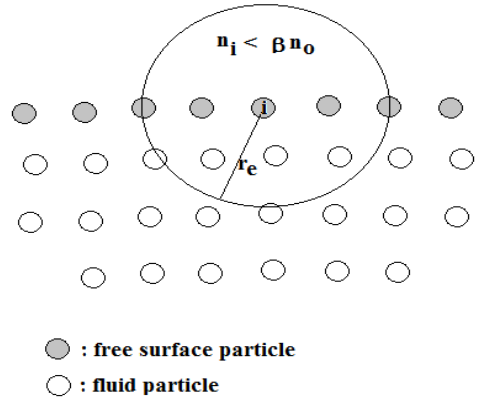


Figure 1. Free surface boundary condition.

In the MPS method, the gradient, the divergence, and the Laplacian models can be calculated by using the following equation:

$$\langle \vec{\nabla}\phi \rangle_i = \frac{d}{n^0} \sum_{j \ne i} \frac{\phi_j - \hat{\phi}_i}{|\vec{r}_j - \vec{r}_i|^2} w\left(|\vec{r}_j - \vec{r}_i|\right) \quad (5)$$

$$\langle \vec{\nabla} \cdot \vec{\varphi} \rangle_i = \frac{d}{n^0} \sum_{j \ne i} \frac{\varphi_j - \varphi_i}{|\vec{r}_j - \vec{r}_i|^2} (\vec{r}_j - \vec{r}_i) w\left(|\vec{r}_j - \vec{r}_i|\right) \quad (6)$$

$$\langle \nabla^2 \phi \rangle_i = \frac{2d}{\lambda n^0} \sum_{j \ne i} (\phi_j - \phi_i) w\left(|\vec{r}_j - \vec{r}_i|\right) \quad (7)$$

In these equations above, d explains the number of spatial dimensions, n^0 explains the initial particle number density, ϕ_j explains the scalar of the j-particle at $\vec{r}_j$, $\hat{\phi}_i$ explains the minimum value of the scalar quantity in the effective radius of the i-target particle, and λ explains the chosen parameter to make the obtained Laplacian model to be proportional to the analytical solution. The value of λ can be determined by using

$$\lambda = \frac{\sum_{j \ne i} w\left(|\vec{r}_j - \vec{r}_i|\right) |\vec{r}_j - \vec{r}_i|^2}{\sum_{j \ne i} w\left(|\vec{r}_j - \vec{r}_i|\right)} \cong \frac{\int_V w(r) r^2 dV}{\int_V w(r) dV} \quad (8)$$

The particle number density with constant value can preserve the incompressible conditions of internal particles where this value decreases for free surface particles. As the free surface particles, the reference particle should achieve the following condition

$$n_i < \beta n^0 \quad (9)$$

where β is the constant value with $\beta < 1$ (1).

Numerical Method

To calculate the equations above, the numerical process is performed. The discritized Laplacian model was utilized to calculate the viscosity term implicitly by using the following approach

$$\vec{u}_k^* = \vec{u}_i^k + \nu \Delta t \frac{2d}{\lambda n^0} \sum_{j \ne i} (\vec{u}_j^* - \vec{u}_i^*) w\left(|\vec{u}_j^k - \vec{u}_i^k|\right) \quad (10)$$

The superscripts * and k represents respectively the temporary value and the value at the last time step. The new temporal velocity with its corresponding position can be determined by using

$$\vec{u}^{**} = \vec{u}^{*} + \Delta t\vec{g} \quad (11)$$

$$\vec{r}^{**} = \vec{r}^{k} + \Delta t\vec{u}^{**} \quad (12)$$

The pressure term of Eq. (2) can be calculated when the Poisson equations of pressure are solved. Both of the corrected velocity and position can be determined by using

$$\vec{u}^{k+1} = \vec{u}^{**} + \Delta t\left(-\frac{1}{\rho^0}\nabla P\right) \quad (13)$$

$$\vec{r}^{k+1} = \vec{r}^{**} + (\Delta t)^2\left(-\frac{1}{\rho^0}\nabla P\right) \quad (14)$$

The flowchart of the used source code can be seen in Figure 2. The Crank-Nicholson method is called to perform the implicit calculation and the finite difference method is invited to perform the explicit calculation.

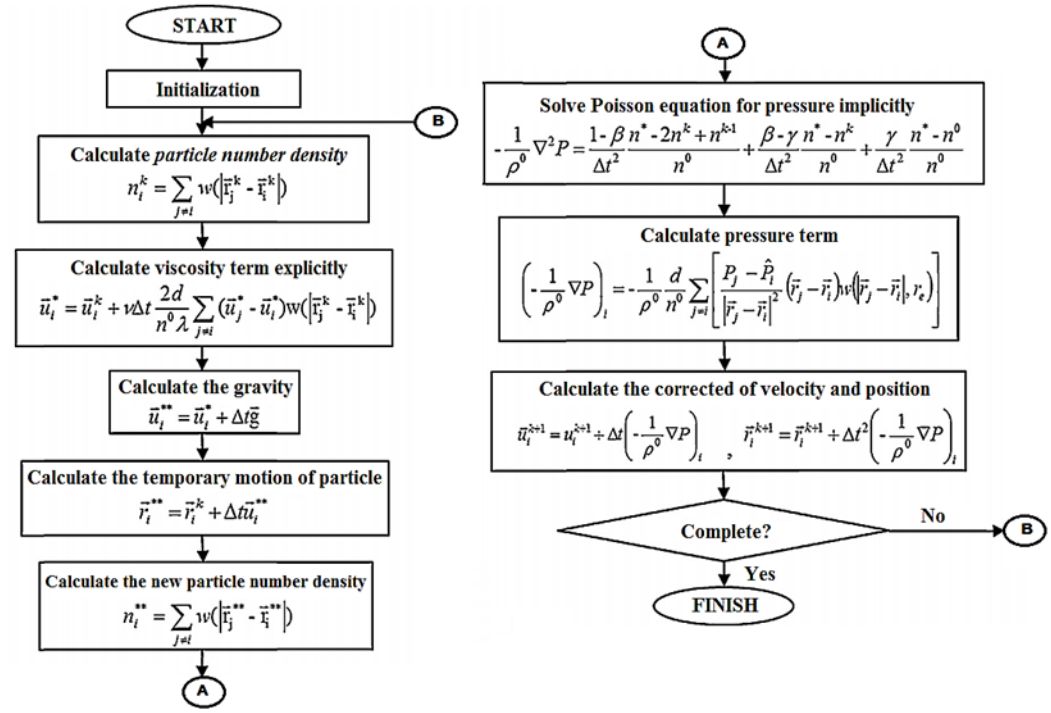


Figure 2. Flowchart of MPS method.

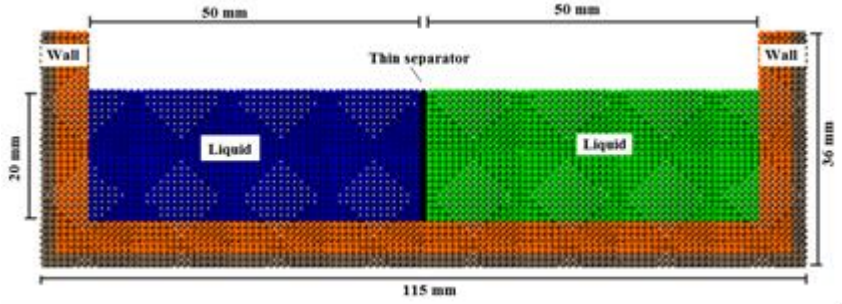


Figure 3. Initial Condition.

Simulation

In this study, it is simulated some materials, i.e. the liquids of PbBi, PbLi, Pb, and Al. The liquids of these materials are miscible chemically. In this study, it is assumed that the stratification process in thermal-hydraulic is faster than in the chemical process as explained in the references (5)(14). Those types of liquids are paired as displayed in Table 1. The initial condition for 2D simulation is shown in Figure 3. The materials were placed inside the containment with 50 mm × 20 mm of size. A thin separator is placed between two liquids. This separator is lifted slowly with 0.2 m/s of velocity. The total used particles are 3231 including the containment wall. The temperature, the density, and the kinematic viscosity of each used material can be seen in Table 1.

Table 1. The parameters of each material (15).

	Component	T (°C)	Density (kg/m^3)	Kinematic viscosity (m^2/s)
Case 1	Pb-Bi	1,000	9.460023×10^3	2.112877×10^{-7}
		1,200	9.210223×10^3	3.409817×10^{-7}
		1,400	8.960423×10^3	5.262757×10^{-7}
	Al	1,000	2.271490×10^3	9.037327×10^{-4}
		1,200	2.209290×10^3	8.295089×10^{-4}
		1,400	2.147090×10^3	7.771429×10^{-4}
Case 2	Pb-Li	1,000	8.848750×10^3	6.065744×10^{-8}
		1,200	8.678750×10^3	5.343103×10^{-8}
		1,400	8.508750×10^3	4.875910×10^{-8}
	Al	1,000	2.271490×10^3	9.037327×10^{-4}
		1,200	2.209290×10^3	8.295089×10^{-4}
		1,400	2.147090×10^3	7.771429×10^{-4}
Case 3	Pb	1,000	9.838934×10^3	9.816614×10^{-8}
		1,200	9.590534×10^3	8.123931×10^{-8}
		1,400	9.342134×10^3	6.835953×10^{-8}
	Al	1,000	2.271490×10^3	9.037327×10^{-4}
		1,200	2.209290×10^3	8.295089×10^{-4}
		1,400	2.147090×10^3	7.771429×10^{-4}

RESULTS AND DISCUSSION

Result

The objective of this study is to observe the stratification process of some materials. The simulation was performed to understand the behavior of the stratification process of those materials. The result of this study is commenced by the stratification process of the PbBi-Al as shown in Figure 4. Next, Figure 5 shows the stratification process of the PbLi-Al. Finally, the stratification process of the Pb-Al is shown in Figure 6. Each stratification process was displayed at three kinds of temperatures, i.e 1,000°C, 1,400°C, and 1,600°C.

Figure 4 shows the mechanism of PbBi-Al stratification, where PbBi penetration faster to the edge of the container. Melted PbBi penetrates and existed below the melted Al. The PbBi reach the edge of the container faster than the Al. As for the other combinations, PbLi and Pb show similar behavior with PbBi in term of reaching the edge, as shown in Figures 5 and 6.

To understand rate of the penetration for each material, time was recorded based on its penetration length in horizontal axis, as shown in Table 2. The length of penetration was determined for 0.6 seconds for each paired material. Figure 7 shows the stratification process based on its penetration by time-step of second between PbBi and Al. It shows that for the three temperatures PbBi penetration reach 50 mm i.e., the edge of the container with similar patterns. The aluminum also shows similar pattern for those three temperatures. Figures 8 and 9 show results of PbLi-Al and Pb-Al at the three temperatures, respectively. Based on the three figures, it can be seen that the penetration patterns are similar for the three combinations, even though the time might vary.

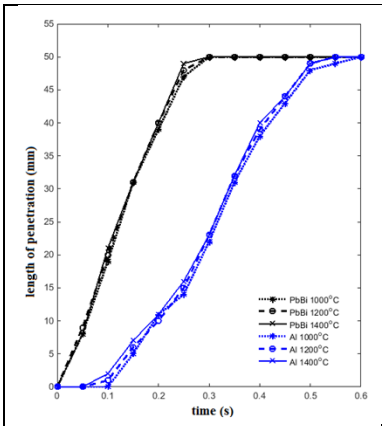


Figure 7. The penetrations of PbBi and Al.

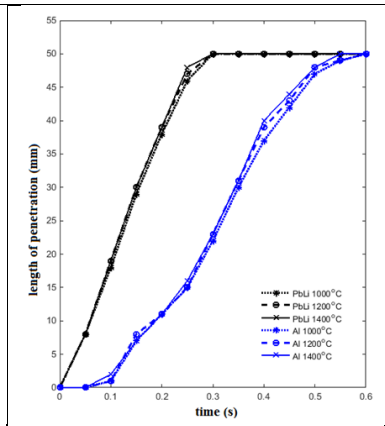


Figure 8. The penetrations of PbLi and Al.

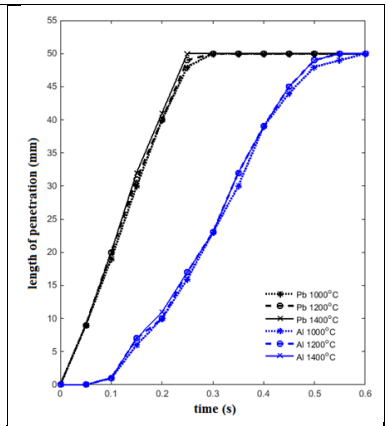


Figure 9. The penetrations of Pb and Al.

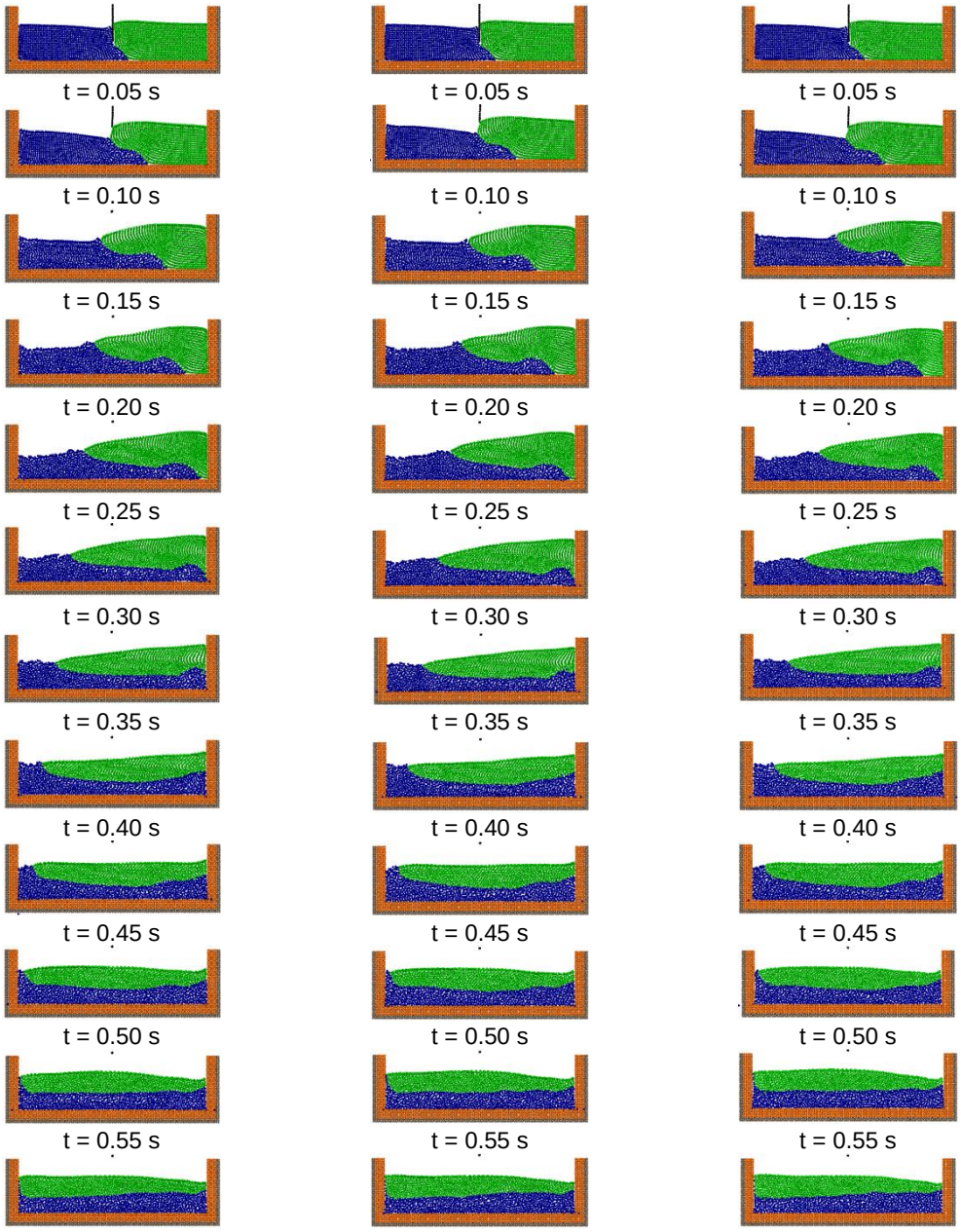
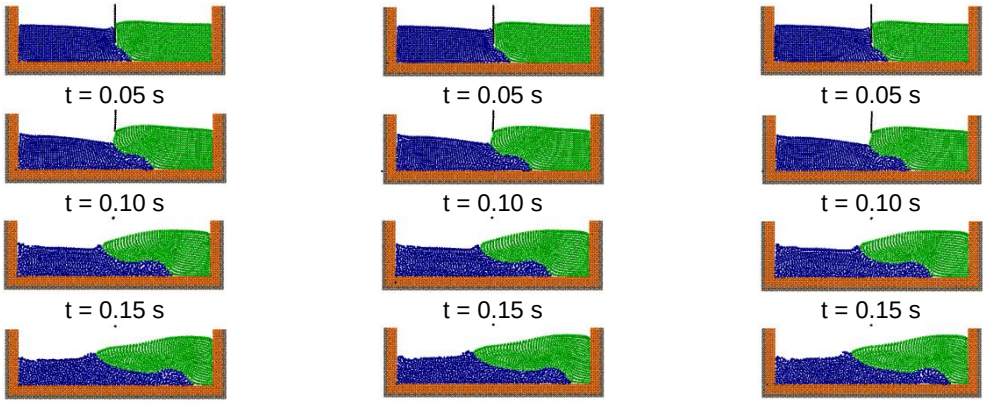


Figure 5. The stratification process of PbLi-Al.



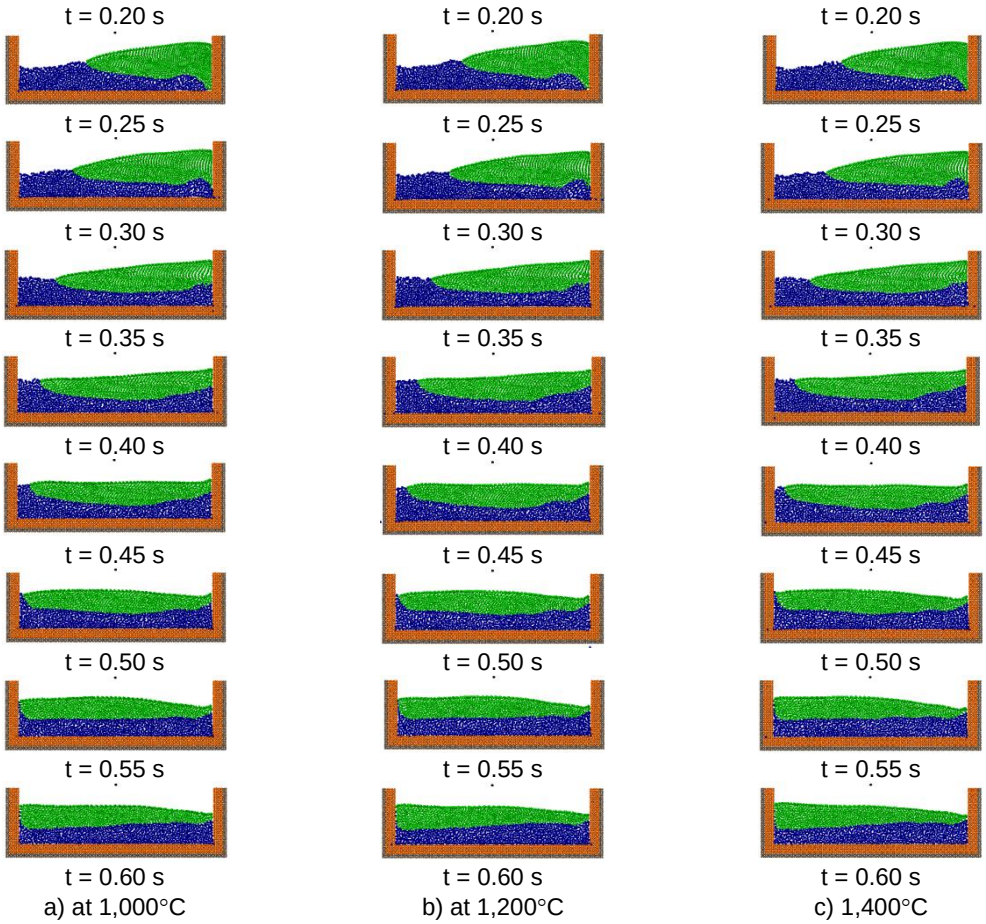


Figure 6. The stratification process of Pb-Al.

Table 1. The length of penetration for each component

	T	Time (s)												
	(°C)	0	0.05	0.1	0.15	0.2	0.25	0.3	0.35	0.4	0.45	0.5	0.55	0.6
	1000	0	8	19	31	39	47	50	50	50	50	50	50	50
Pb-Bi	1200	0	9	20	31	40	48	50	50	50	50	50	50	50
	1400	0	8	21	31	40	49	50	50	50	50	50	50	50
	1000	0	0	0	5	11	14	22	31	38	43	48	49	50
Al	1200	0	0	1	6	10	15	23	32	39	44	49	50	50
	1400	0	0	2	7	11	16	23	32	40	44	49	50	50
	1000	0	8	18	29	38	46	50	50	50	50	50	50	50
Pb-Li	1200	0	8	19	30	39	47	50	50	50	50	50	50	50
	1400	0	8	19	20	39	48	50	50	50	50	50	50	50
	1000	0	0	1	7	11	15	22	30	37	42	47	49	50
Al	1200	0	0	1	8	11	15	23	31	39	43	48	49	50
	1400	0	0	2	7	11	16	23	31	40	44	48	50	50
	1000	0	9	19	30	40	48	50	50	50	50	50	50	50
Pb	1200	0	9	20	31	40	49	50	50	50	50	50	50	50
	1400	0	9	20	32	41	50	50	50	50	50	50	50	50
	1000	0	0	1	6	10	16	23	30	39	44	48	49	50
Al	1200	0	0	1	7	10	17	23	32	39	45	49	50	50
	1400	0	0	1	7	11	17	23	32	39	45	49	50	50
		Length of penetration (mm)												

Discussion

The results above show the stratification process for each material at three different temperatures. For the same combination, each temperature shows similar result to each other. From figures above, it can be seen that each material combinations needs about 0.5 seconds to reach the stratified condition. However, the result is a little different when the combination ~~is~~ was changed. It is shown that the stratification time for Pb-Al is the fastest among the combinations, followed by PbBi-Al then PbLi-Al in the third place. It seems that the temperature gives little effect to the stratification process. The time to reach the stratified condition is influenced significantly by the difference in density between two liquids. The greater the difference in density between two liquids, the faster the achievement of stratified condition. However, since the simulation temperatures are high the results may show differently at probably lower temperature. Thus, further investigation is needed to conclude that the temperature effect is minor.

The results of this study are still in the early stages, it is expected that further research is able to compare the numerical simulations with the relevant experiments. On the other hand, to make the research more quantitative, future studies can be extended to investigate the stratification of two (or more) liquids with different viscosities or densities or temperatures or different initial configurations.

CONCLUSION

The stratification behavior of some combination materials has been investigated in this study. In this study, it is simulated some materials, i.e. the liquids of PbBi, PbLi, Pb, and Al. The MPS method has been utilized to simulate the stratification process of these materials. From the obtained figures, it can be seen each material combination needs 0.5 seconds to reach the stratified condition. The obtained results show that the Pb-Al is the fastest to reach the stratified condition among the other used materials. It means that the difference in density between two liquids influences the time to attain the stratified condition. The greater the difference in density between two liquids, the faster the stratification process. For improving the quantity of study, it is very important that further studies are capable of collaborate the numerical simulations with the relevant experiments.

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