Moving Particle Semi-implicit (MPS) Utilization in Analyzing the Stratification Behavior of Immiscible Liquid

Y Yulianto¹, A N Hidayati¹, A P A Mustari²*, M Ilham¹ and S Pramuditya²

¹Magister Program of Physics Department, Faculty of Mathematics and Natural Science, Bandung Institute of Technology, Jalan Ganesha 10, Bandung 40132, Indonesia
²Nuclear Physics and Biophysics Research Division, Physics Department, Faculty of Mathematics and Natural Science, Bandung Institute of Technology, Jalan Ganesha 10, Bandung 40132, Indonesia

*pramutadi@fi.itb.ac.id

Abstract. The reactor core accident, especially the reactor core melt-down, is one of the most important things to be considered in analyzing the reactor safety factor. In melted reactor core case, one of the interesting phenomena which can be examined is the process of stratification of a metallic liquid component of the melted reactor core. In this study, it is observed the stratification process of immiscible liquid through simulation and validation with experiment. One method that can be utilized to model the liquid stratification is the MPS (Moving Particle Semi-Implicit) method. The stratification experiments were conducted using water and several kinds of oils. From the gained results, it can be seen that the obtained results of the simulation are in good agreement with the experiment results. In addition, from the simulation and experimental results, it can be seen that the density of liquid significantly affects the stratification process. The kinematic viscosity of liquid also affects the rate of liquid penetration in achieving stratification conditions. Therefore, the MPS method used in this simulation has a good enough capability to simulate the liquid stratification phenomena, which can be implemented in conditions of the melted reactor core prototype.

1. Introduction

Although the usage of nuclear technology in providing an energy source has a significant development, it also faces many problems to be solved. Reactor core accidents (Chernobyl, Three Miles Island, and Fukushima) have made us consider seriously about reactor safety. One of the core accidents is heat accumulation in reactor core because of uncirculated coolant (loss of coolant accident). Therefore, it is needed a study to explain the behavior of melted reactor materials when reactor core accidents occur. The experiment is insufficient for some special conditions. In the other hand, the conventional simulation methods, independent of empirical correlations, also have difficulty to analyze several melted core phenomena, such as free-surface flow, phase transition, and stratification. One of the methods that can be utilized to simulate the melted core phenomena is Moving Particle Semi-Implicit (MPS) method, introduced initially by Koshizuka and Oka [1]. This MPS method, which has been applied in nuclear engineering [2-6] and ocean engineering [7-10], is a particle method that can be used to analyze incompressible free surface flow, with messless.
In this study, the original MPS source code has been modified to simulate stratification behavior of two immiscible liquids. For verifying, it was observed by using experiment with three different immiscible liquids, i.e., water, cooking oil, and lubricant oil. The effects of both density and kinematic viscosity liquids have also been investigated by using simulation.

2. Model and numeric simulation

2.1. Governing equation

The governing equation for incompressible flow used commonly is Navier-Stokes equation, which can be formulated as [5,10,11]

\[
\frac{D\rho}{Dt} = 0
\]

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

where \(\rho\) represents the density, \(t\) represents the time, \(\vec{u}\) represents velocity vector, \(\nu\) represents the gradient, \(P\) represents the pressure, \(\nu\) represents the kinematic viscosity, and \(\vec{g}\) represents gravity.

2.2. Moving Particle Semi-Implicit (MPS) method

The MPS method is a meshless particle method to analyze incompressible flow. Particle interaction is defined according to its position related to the reference particle. The particle motion can be calculated from interaction force between two nearest particles by using weight function related to the distance. The commonly used weight function of MPS method can be formulated by:

\[
w(r) = \begin{cases} 
(1 - \frac{r}{r_e})^2 & 0 \leq r \leq r_e \\
0 & r_e \leq r 
\end{cases}
\]

where \(r\) is the distance between two particles and \(r_e\) is the cut-off radius for limited interactions [1,5]. The weight function approaches to be zero when the distance between two particles is higher than the cut-off radius [1], as shown in Figure 1 and Figure 2.

![Figure 1. Weight function [5].](image1)

![Figure 2. Free surface boundary condition [5].](image2)

The particle number density, which equals to the liquid density, on the i-particle position can be written as

\[
n_i = \sum_{j \neq i} w(|\vec{r}_j - \vec{r}_i|)
\]

Where \(\vec{r}_i\) and \(\vec{r}_j\) are position vectors of \(i\) and \(j\) particles [5,10,12,13]. The gradient, divergence, and Laplacian models can be calculated by using:

\[
(\nabla \phi)_i = \frac{d}{n^0} \sum_{j \neq i} \frac{\phi_j - \phi_i}{|\vec{r}_j - \vec{r}_i|^2} w(|\vec{r}_j - \vec{r}_i|)
\]
\[
\langle \nabla, \varphi \rangle_i = \frac{d}{n^0} \sum_{j=1}^{n^0} \frac{\varphi_j - \varphi_i}{|\vec{r}_j - \vec{r}_i|^2} (\vec{r}_j - \vec{r}_i)w(|\vec{r}_j - \vec{r}_i|)
\]

\[
\langle \nabla^2 \varphi \rangle_i = \frac{2d}{\lambda n^0} \sum_{j=1}^{n^0} (\varphi_j - \varphi_i)w(|\vec{r}_j - \vec{r}_i|)
\]

Where \(d\) is the number of spatial dimensions, \(n^0\) represents the initial particle number density, \(\varphi_i\) represents the scalar of the \(j\)-particle at \(\vec{r}_i\), \(\phi_i\) is the minimum value of the scalar quantity in the effective radius of the \(i\)-target particle, and \(\lambda\) is the parameter chosen to make the obtained Laplacian model to be proportional to the analytical solution [13,14]. The value of \(\lambda\) can be approximated by

\[
\lambda = \frac{\sum_{j=1}^{n^0} w(|\vec{r}_j - \vec{r}_i|)|\vec{r}_j - \vec{r}_i|^2}{\sum_{j=1}^{n^0} w(|\vec{r}_j - \vec{r}_i|)} \cong \frac{\int_V w(r)r^2dV}{\int_V w(r)dV}
\]

The particle number density is set to be constant for the internal particles to preserve the incompressible conditions, while it decreases for the particles located on the free surface. The observed particles, regarded as free surface particles shown in Figure 2, should meet the condition of

\[
n_i < \beta n^0
\]

Where \(\beta\) is the constant value which satisfies \(\beta < 1\) [1,5]. In this study, viscosity term was first implicitly calculated by using the discretized Laplacian model [5].

\[
\vec{u}_k = \vec{u}_i^k + v \Delta t \frac{2d}{\lambda n^0} \sum_{j=1}^{n^0} (\vec{u}_j - \vec{u}_i)w(|\vec{u}_j - \vec{u}_i|)
\]

Where the superscript * and k represent respectively the temporary values and the values at the last time step. Furthermore, new temporal velocity and its corresponding position can be obtained by [5]

\[
\vec{u}^* = \vec{u} + \Delta t \vec{g}
\]

\[
\vec{r}^* = \vec{r} + \Delta t \vec{u}^*
\]

Pressure term on the eq. (2) is calculated after solving the Poisson equation of pressure. However, velocity and position are corrected by using [5].

\[
\vec{u}^{k+1} = \vec{u}^* + \Delta t \left( - \frac{1}{\rho \nu} \nabla P \right)
\]

\[
\vec{r}^{k+1} = \vec{r}^* + (\Delta t)^2 \left( - \frac{1}{\rho \nu} \nabla P \right)
\]

The flowchart of the source-code used in this study can be seen in Figure 3, where all calculations of left side were performed explicitly by using the finite difference method and all calculation of right side were performed implicitly by using Crank-Nicholson method.

2.3. Experiment and simulation

In this study, stratification experiments were performed by using two combinations of immiscible liquids placed on a 40 \(\times\) 40 \(\times\) 50 mm container with a thin separator. The height of the liquid was 30 mm from the bottom of the container. Each container was filled with two types of liquids with 30 mm of height. Observations were made for three different liquids, as presented in Table 1.

In Figure 3 and Figure 4, the initial particle in 2D for stratification process of two different liquids with 1 mm of separator thickness. The total of particles of each liquid was 1200, and the total of used particles (including the parts of the container and separator) was 3249. The velocity of the separator is 0.2 m/s until the entire separator is lifted and does not touch the liquid. When dealing with particles located on the liquid interface, the viscosity, and density used in the calculations are the average values.
of each used liquids. The solid boundary condition between the liquid and the wall is assumed not to slip. The used liquid parameters, obtained from [15,16], can be seen in Table 1.

| Parameter                  | Case A  | Case B  | Case C  |
|----------------------------|---------|---------|---------|
|                            | Liquid 1| Liquid 2| Liquid 1| Liquid 2| Liquid 1| Liquid 2|
| Liquid 1                   | Cooking oil| Freshwater| Lubricant oil| Freshwater| Cooking oil| Lubricant oil|
| Density (kg/m³)            | 890.13  | 1000    | 848.30  | 1000    | 890.13  | 848.30    |
| Kinematic viscosity (mm²/s)| 53.146  | 1.004   | 143.70  | 1.004   | 53.146  | 143.70    |

Table 1. Liquid parameters.

![Flowchart of MPS method](image)

Figure 3. Flowchart of MPS method [14].

![Set up of particles in initial condition for liquid stratification experiments](image)

Figure 4. Set up of particles in initial condition for liquid stratification experiments.

3. Results and Discussion

In this study, experiments were carried out first. After the experimental data obtained, it continued with simulation. From Figure 5, it can be seen a side view of the experiment and simulation results for cooking oil and water, with the process of that liquid to reach stratified condition, where the results obtained by the simulation are faster than those of the experiment, but the patterns toward the stratified condition are quite similar. It is similar to Figure 6, the stratification process of lubricating oil and water.
Unlike the case when heading to figure 7, the stratification process of cooking oil-lubricating oil. The obtained results are entirely different from the obtained results in Figures 5 and 6. From Figure 7, the obtained results of the simulation are somewhat slower than those of experiment. However, the pattern toward stratification condition is sufficiently similar to the experiment. This is because the difference density between cooking oil and lubricating oil is not so significant so that the obtained pressure gradient becomes small which further causes the liquid moves slowly. By that, the difference in inter-liquid density is one of the essential things in stratification.

\[ a) \ t = 0.18 \text{ second} \]

\[ b) \ t = 0.52 \text{ second} \]

\[ c) \ t = 1.00 \text{ second} \]

\[ d) \ t = 1.48 \text{ second} \]

**Figure 5.** Side view of the experiment (left) and simulation (right) for cooking oil and water.

In this study, it is also calculated the ratio of the breakthrough distance of each liquid to observe the kinematic viscosity effect on the rate of penetration. In Figure 8, it appears that at first, the process of water breakthrough was faster than the breaking of cooking oil, but not significantly. In addition, faster simulation results achieve stratification condition than experimental results. The results are also similar to those of lubricating oils and water, as shown in Figure 9.

In Figure 10, it appears that the experiment results were the first which reached the stratified condition. This is predicted because some parameters are not suitable to simulate the case of lubricant oil and cooking oil. Therefore, the need for further analysis in the used script-code or given input. Figure 11 shows the time it takes for water to infiltrate into the oil faster than when infiltrated in the lubricating oil. This result explains that the higher the kinematic viscosity of the liquid, the more difficult to be infiltrated.
Figure 6. Side view of the experiment (left) and simulation (right) for lubricant oil and water.

Figure 7. Side view of the experiment (left) and simulation (right) for lubricant oil - cooking oil.
Based on the gained results, it can be seen that the liquid density dramatically influences the stratification pattern, where the liquid that has larger density is under the liquid that has smaller density. In addition, significant density differences (the difference density of two liquids) can cause substantial pressure gradient that causes the velocity induced by the pressure gradient to increase and subsequently cause the liquid to move faster. It means that the difference density between two liquids is one of the essential things in stratification investigation.

In addition, time to reach the stratified condition is also influenced by the liquid viscosity. More viscous the liquid (has high kinematic viscosity), more difficult it to be penetrated, so it takes a long time to reach the stratification condition.

**Figure 8.** The ratio of penetration length for cooking oil and water.

**Figure 9.** The ratio of penetration length for lubricant oil and water.

**Figure 10.** The ratio of penetration length for lubricant oil and cooking oil.
4. Conclusions

In this study, both simulation and experiment have been carried out to analyze the stratification behavior of immiscible liquids. Original MPS source-code has been developed by incorporating implicit viscosity calculation models and stability improvement models to simulate the stratification behavior of liquids with high kinematic viscosity. In this study, the stratification behavior of three different immiscible liquids has been investigated through simulation by using the MPS method. The simulation results have been validated by using experiments, where the results obtained through the simulation are quite similar to the results obtained through the experiment. The results obtained show that the liquid viscosity and the difference in density between the two liquids significantly affect the liquid configuration and the time required to reach the stratified condition. In addition, the higher the kinematic viscosity of the liquid, the harder it is to break through. The simulation results in 2D show good suitability with the experiment, which shows that the modified MPS source-code has the ability to analyze the phenomenon of liquid stratification, which can be implemented under the melted condition of the reactor core prototype.

Acknowledgment
This study is fully funded by Ministry of Research, Technology, and Higher Education 2017, Indonesia.

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