Experimental research and numerical simulation of moving molten metal pool

Penghui CHAI*, Nejdet ERKAN**, Masahiro KONDO**, Koji OKAMOTO** and Hongyang WEI*
*Department of Nuclear Engineering and Management, The University of Tokyo
Hongo 7-3-1, Bunkyo ku, Tokyo 113-8654, Japan
E-mail: phchai@vis.t.u-tokyo.ac.jp
**Nuclear Professional School, The University of Tokyo
Hongo 7-3-1, Bunkyo ku, Tokyo 113-8654, Japan

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Abstract
Plenty of numerical simulations were performed to analyze the Molten Core-Concrete Interaction (MCCI) phenomena since 1980s. However, uncertainties remain among thermal hydraulic codes. Thus, in order to avoid the effect of uncertainties due to the different empirical formulas and interfacial models, a new CFD code based on Moving Particle Semi-implicit (MPS) method was proposed to simulate the MCCI event in the literature. Validation of the heat transfer and phase-change models is still necessary to utilize MPS method for the MCCI modeling. In this study, a small-scale visualization experiment was conducted using melted hot u-alloy and solid transparent gel wax to acquire quantitative data for validating heat transfer and phase change models of MPS method. Comparison of the simulation and experimental results demonstrates good agreement on ablation behavior and deformation profile of the molten metal moving downwards by the phase change of wax. Additionally temperature evolution in time showed consistency with the thermocouple measurements. Obtained results suggest that MPS code have capacity to simulate the phase change and heat transfer mechanisms of moving molten metal pool which are important mechanisms for the MCCI event.

Key words: MCCI, MPS, Phase change, Validation, Molten metal, Wax

1. Introduction

Molten Core-Concrete Interaction (MCCI) takes place after early pressure vessel failure. It may results in catastrophic large fission product release and land contamination due to containment failure, which results from the pressurization with the large amount of gas generation during the corium-concrete interaction and the melt-through of the basemat. Therefore, MCCI and concrete ablation should be investigated diversely. A number of MCCI experiments were performed since 1980s (H. Alsmeyer et al; 1995, Copus, 1992; Copus et al., 1989, 1990; D.H. Thompson et al., 1997; M.T.Farmer et al., 2006). Most experiments produced the expected results and provided many important findings. However, due to the limitation of the measurement techniques under the extreme experimental conditions, some transient data could not obtained from the experiment results. Thus, numerical simulation is seems as a proper way to explore the detail MCCI phenomena, as well as to predict the MCCI sequence in the real nuclear power plant.

Plenty of thermal hydraulic codes with empirical interfacial models were developed to simulate the MCCI process. Such as ASTEC/MEDICIS, WECHSL, MELCORE (Cranga et al., 2008, 2010; Farmer, 2001; Foit, 1995; Strizhov, 1996). Different heat transfer correlations between concrete and corium were applied, as well as the interface model on the crust area and the concrete ablation model. Based on the benchmark results, large deviations existed in predicting the ablation shape and average temperature of the corium, which was due to the different empirical interfacial models were applied (Cranga et al., 2010). This points to limitations in empirical formula application in MCCI simulation, and indicates the necessity to develop a code in which only fundamental governing equations are used in order to understand the mechanics of the interaction phenomena.

Consequently, Moving Particle Semi-implicit (MPS) method is considered as a candidate tool to analyze MCCI phenomena. The MPS method (Sheu et al., 2011; Zhang 2005; Yoon et al., 1999) is one of the particle methods based on
the Lagrangian description, which was initially developed by Koshizuka and Oka (1996) in 1990s. The most important merit of the MPS method in investigating the MCCI process is that large deformations of interfaces can be analyzed without grid tangling and numerical diffusion because the convection terms are directly calculated by the motion of the particles. Numerous research efforts successfully utilized the MPS method to analyze the complex motion of free surfaces, such as the collapse of water columns (Koshizuka and Oka, 1996) and breaking waves (Koshizuka et al., 1998). Thus, the MPS method is a potential proper tool to analyze the mechanistic of phenomena in the MCCI process.

Prior to the simulation of a complex phenomenon, it is essential to validate and quantify the applicability of each models for such a moving molten metal pool simulation. As a first step, heat transfer and phase change models, which form the fundamental mechanisms of the MCCI, should be validated. The heat transfer and phase change models were originally developed and implemented in the MPS by Koshizuka (1996). Recently, MPS method was applied for the simulation of eutectic melting or other complicated phenomena, which contain highly coupled physical mechanisms with existing phase change and heat transfer models. Chen et al (2014a; 2014b) analyzed the freezing behavior with empirical viscosity model, which is highly dependent on an empirical parameter. Pramutadi et al (2014) developed the eutectic model and validated against experiments without heat transfer. Li et al (2014a; 2014b) analyzed the corium spreading and stratification behavior in the pressure vessel lower head, while surface tension was ignored even tough two immiscible fluids were modelled. The results of the validations mentioned above are hard to evaluate to be able to obtain a refined idea due to the discrepancies between the simulation and experimental results since the complex problems contains substantial interacting mechanisms incorporated with numerous parameters. Thus, some fundamental mechanisms implemented in the MPS method should be assessed and validated against separate effect tests to assure the accuracy with isolating or reducing interrelated parameters.

For that purpose, in this paper, a small-scale experiment with a metallic alloy having low melting temperature was performed to reproduce the molten metal behavior at low temperature conditions with surface tension for the validation of the heat transfer and phase change models of the MPS code. Gel wax is chosen to be ablated because of its transparent properties so that the erosion process can be visualized. The MPS code is applied to simulate this experiment and the results compared to validate the models.

2. Numerical method

2.1 Basic MPS method

The governing equations of the MPS method are the continuity, Navier-Stokes, and energy conservation equations:

\[ \nabla \cdot \mathbf{u} = 0 \quad (1) \]

\[ \frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} = -\frac{1}{\rho} \nabla p + \nu \nabla^2 \mathbf{u} + \mathbf{F} \quad (2) \]

\[ \frac{\partial h}{\partial t} = k \nabla^2 T + Q \quad (3) \]

where \( \rho \), \( t \), \( \mathbf{u} \), \( p \), \( \nu \), \( \mathbf{F} \), \( k \), \( h \), \( T \), and \( Q \) are density, time, velocity vector, pressure, kinematic viscosity, external force, enthalpy, thermal conductivity, temperature, and heat source, respectively.

More detailed explanation of the MPS algorithm can be found in (Koshizuka et al., 1998, 1996).

2.2 Heat transfer, phase-change and surface tension models

Heat transfer between particles is discretized based on the energy equation (Eq. 3). The equation can be explicitly solved using the Laplacian model:

\[ \frac{Dh}{Dt} = \frac{2d}{n^2 \lambda} \sum_{j=1}^{n} \left[ k_j (T_j - T_i) \right] v \left( |r_j - r_i| \right) + Q \quad (4) \]
where $h$ and $Q$ are the enthalpy and heat source of particle $i$, respectively. Temperature can then be calculated from enthalpy $h$.

$$T = \begin{cases} 
T_i + \frac{h-h_i}{\rho C_{ps}} & (h < h_i) \\
T_i + \frac{h-h_i}{h_i-h_s} (T_s - T_i) & (h_i \leq h \leq h_l) \\
T_i + \frac{h-h_i}{\rho C_{pl}} & (h < h_l)
\end{cases}$$

(5).

where $T_s$, $T_l$, $h_s$, $h_l$ are solidus temperature, liquidus temperature, the solid enthalpy at the melting point and the liquid enthalpy at the melting point, respectively.

To express the phase change, solid-fraction $\gamma$ is introduced and calculated based on enthalpy $h$ using

$$\gamma = \begin{cases} 
1 & (h < h_i) \\
\frac{h_i-h}{h_i-h_s} & (h_i \leq h \leq h_l) \\
0 & (h < h_l)
\end{cases}$$

(6), which is used as a criterion to judge the phase of the material.

Surface tension model implemented in this research is originally developed by Kondo et al. (2007), where potential force between the interface particles was used to simulate the surface tension. The detail algorithms can be found in (Kondo et al., 2007).

### 3. Experimental set up and approach

A schematic view of the experimental apparatus is shown in Fig. 1. The gel wax was contained in a transparent glass container with dimensions 7 cm × 7 cm × 6 cm. Initially, u-alloy was heated in the hotpot to 190°C, while the temperature of the gel wax was 20°C. Then, the melted u-alloy was poured into the cylindrical cavity at the center of the pool made of gel wax. Ablation immediately began after the pouring. The ablation movement was captured by a high-speed camera at a rate of 2 fps. The temperature was measured with three K-type thermal-couples at locations (-1.0 cm, 0.5 cm), (-1.0 cm, 1.8 cm), and (0 cm, 3.5 cm). The data acquisition was carried out using a data logging system at a frame rate of 1 fps.

![Fig. 1 Principle-view of the experimental apparatus](image-url)
4. Simulation configuration

A two-dimensional domain was established to simulate the experiment by the MPS method, as shown in Fig. 2. There are three types of particles, represented by blue, green, and red. They are u-alloy particles, gel-wax particles, and wall particles, respectively. The wall particles were only used to calculate the particle number densities. Since they did not exchange heat with the inner particles, the wall was adiabatically modeled in this simulation. To express the phase change of the gel wax, each gel-wax particle was judged to be either fluid or solid using Eq. 7 in every time step. The fluid particles’ movement was calculated by solving the momentum equation, while the solid particles were fixed in the previous position. The initial simulation condition is shown in Table 1, and the material properties (Ukrainczyk et al., 2009; Yuanyuan and Xiaoming, 2013) used in the code are shown in Table 2.

Fig. 2 Initial particle configuration

Table 1. Initial condition of the simulation

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Initial temperature of gel wax (K)</td>
<td>293.0</td>
</tr>
<tr>
<td>Initial temperature of u-alloy (K)</td>
<td>464.0</td>
</tr>
<tr>
<td>Average distance between particles (m)</td>
<td>0.001</td>
</tr>
<tr>
<td>Total number of particles</td>
<td>9126</td>
</tr>
</tbody>
</table>

Table 2. Physical properties of materials utilized

<table>
<thead>
<tr>
<th>Property</th>
<th>U-alloy</th>
<th>Gel wax</th>
<th>Glass</th>
</tr>
</thead>
<tbody>
<tr>
<td>ρ [kg/m³]</td>
<td>9580.0</td>
<td>3550.0</td>
<td>2300.0</td>
</tr>
<tr>
<td>Thermal conductivity [W/m·K]</td>
<td>36.0</td>
<td>0.4</td>
<td>1.09</td>
</tr>
<tr>
<td>Specific heat [J/(kg·K)]</td>
<td>790.0</td>
<td>780.0</td>
<td>600.0</td>
</tr>
<tr>
<td>Latent heat [J/kg]</td>
<td>45800.0</td>
<td>43700.0</td>
<td>-</td>
</tr>
<tr>
<td>Melting temperature [°C]</td>
<td>70.0</td>
<td>50.0</td>
<td>2000.0</td>
</tr>
</tbody>
</table>

5. Results and discussion

The profile of the metal deformation process in the experiment can be seen in the pictures in Fig. 3. The process can be divided into two main stages. From the very beginning to around 80 s, the ablation process is nearly homogenous.
because of the uniform temperature distribution of the melt pool. In addition, crust is generated after around 60 s in the bottom of the melt, which reduces the heat transfer between the molten metal and gel wax. The second stage is from 80 s; molten metal gains its final shape after some time and continues its downward motion while preserving its shape. This is because the u-alloy is cooled down by the gel; the surface temperature goes down below the solidification point of the u-alloy. Therefore, a shell is gradually generated and surrounds the melting material. However, the ablation process does not stop because the surface temperature is still higher than the melting point of gel wax. The final melting depth in the central line was 2.2 cm.

Fig. 3 Ablation process and metal deformation along the elapsed time. (First line, from left to right: 5 s, 20 s, 40 s; Second line, from left to right: 60 s, 80 s, 100 s.)

Figure 4 is a series of pictures that compares the ablation profile between the simulation and the experiment at three time points. In order to clearly compare the molten metal deformation process with the experiment, the particles are represented by their material type. From the pictures, it is clear that the ablation profile simulated by the MPS method is congruent with the experiment.
Figure 5 compares the erosion front head, with both axial and radial direction, of the experiment and the MPS method. A good agreement on both the downward and sideward ablation can be seen in the picture. The liquid metal melted the wax almost homogenously. The ratio of axial and lateral ablation at time=100.0s is 1.27, which is very close to the value in the experimental results. The ablation speed gradually decreased in both experiment and the MPS simulation.

![Graph showing erosion depth over time](image)

Figure 5 Erosion front head during the ablation process

Figure 6 is a series of pictures showing the temperature distribution of the whole region with elapsed time in the simulation. It can be seen from the pictures that the temperature of u-alloy decreased since it was cooled down by the gel wax. In addition, a very small temperature diffusion appears as a result of the low thermal conductivity of gel wax.

![Temperature changes with elapsed time](image)

Fig. 6 Temperature changes with elapsed time

Figure 7 gives a comparison of the temperature measured by the thermocouples and the temperature calculated by...
the MPS method at the same place. It can be seen that in the experiment, the temperature of the top thermocouple decreased rapidly for the first 30 s, which is because the u-alloy is cooled down by the gel wax during the process of being poured into the cavity. The molten pool reached the second thermocouple at 58 s in the simulation, which was slightly earlier than that in the experiment. Further, the temperature of the second thermocouple rises rapidly because of the low temperature diffusion of gel wax. The curve of the experiment changes gently, probably because there was some gel wax remained around the thermocouple when it was heated by the molten pool, and results in deceleration of the melting process in the location of the second thermocouple. All in all, although deviation exists, the value and tendency is mainly matches the experiment.

![Temperature of the thermocouples](image)

**Fig. 7 Temperature of the thermocouples**

### 6. Conclusion

A validation study was performed for the mass and heat transfer modelling of the MPS method. A small-scale experiment using u-alloy and gel wax was conducted in order to visualize the erosion process and to obtain the data for the code validation.

From the visualization, the motion of molten metal can be classified into mainly 2 stages: From the very beginning to around 80 s, the ablation process is nearly homogenous because of the uniform temperature distribution of the melt pool. After 80 s, molten metal gains its final shape after some time and continues its downward motion while preserving its shape.

The experiment was simulated by using the developed MPS code with added surface tension model. Deviation exists in the temperature history when the hot corium pouring into the pool. On the other hand, ablation behavior and deformation profile of the molten metal matched the experimental results relatively better.

The overall findings suggest that the MPS code is applicable to the simulation of the moving molten metal pool. Therefore, MPS method has potential capability to model mass and heat transfer mechanisms prevalent in a real MCCI event.

### References


