Development of MPS Method for Analyzing Melt Spreading Behavior and MCCI in Severe Accidents

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Abstract. Spreading of molten core (corium) on reactor containment vessel floor and molten corium-concrete interaction (MCCI) are important phenomena in the late phase of a severe accident for assessment of the containment integrity and managing the severe accident. The severe accident research at Waseda University has been advancing to show that simulations with moving particle semi-implicit (MPS) method (one of the particle methods) can greatly improve the analytical capability and mechanical understanding of the melt behavior in severe accidents. MPS models have been developed and verified regarding calculations of radiation and thermal field, solid-liquid phase transition, buoyancy, and temperature dependency of viscosity to simulate phenomena, such as spreading of corium, ablation of concrete by the corium, crust formation and cooling of the corium by top flooding. Validations have been conducted against experiments such as FARO L26S, ECOKATS-V1, Theofanous, and SPREAD for spreading, SURC-2, SURC-4, SWISS-1, and SWISS-2 for MCCI. These validations cover melt spreading behaviors and MCCI by mixture of molten oxides (including prototypic UO2-ZrO2), metals, and water. Generally, the analytical results show good agreement with the experiment with respect to the leading edge of spreading melt and ablation front history of concrete. The MPS results indicate that crust formation may play important roles in melt spreading and MCCI. There is a need to develop a code for two dimensional MCCI experiment simulation with MPS method as future study, which will be able to simulate anisotropic ablation of concrete.

1. Introduction

In a postulated severe accident of a light water reactor (LWR), behavior of core melt (mixture of molten core and structural materials) determines progression and consequence of the accident. While in-vessel retention (IVR) of molten core (corium) is desirable from the viewpoint of accident management, eventual failure of a reactor pressure vessel (RPV) may be inevitable for the current LWRs and some of the advanced LWR designs if core cooling cannot be recovered [1]. Hence, discharge of corium into the reactor cavity and spreading on the containment concrete basemat are expected in the late phase of an LWR severe accident, leading to molten core concrete interaction (MCCI). If sufficient amount of corium is accumulated on the basemat without any mitigation measures, the corium may gradually ablate through the basemat and the walls of the reactor pit and may lead to release of large amount of fission product (FP) to the environment.

Hence numerous experiments have been conducted and various simulation codes have been developed and validated against experiments to understand the melt spreading behavior and MCCI. However, many of these codes exhibited difficulties of tracking free surface and calculating
temperature profile of the melt without use of empirical equations obtained from experiments [2-4]. There were large uncertainties among different codes in predicting axial and lateral concrete ablations during MCCI [5-9]. Moreover, there is only preliminary understanding about mitigation and termination of MCCI by water flooding [5, 10]. Hence, understanding of these melt spreading behavior and MCCI need further improvement.

One of the key aspects of simulating melt spreading and MCCI is tracking of free surface throughout the analysis. Simulation codes used in the above mentioned studies are based on Eulerian method and exhibit difficulties with the tracking. For example, Finite Element Methods (FEM) have difficulties with large distortions of meshes and Volume Of Fluid (VOF) methods tend to encounter numerical divergence at the boundary of free surface when simulating large deformation of free surface. In contrast, Lagrangian method is much more suitable for tracking free surface motions. Moving Particle Semi-implicit (MPS) method is one of the particle methods for incompressible flow and is based on a Lagrangian method [11]. In this method, continua like fluid can be expressed by calculation points (particles) and motions of free surfaces can be easily tracked by movement and interaction models of the particles (calculating points). Thus, empirical correlations, as often adopted by Eulerian methods, are not necessary in tracking the free surface.

The MPS method has been extensively studied and developed for simulations of different phenomena involved in severe accident of nuclear reactors, such as eutectic melting of metals[12], phase change and stratification of melts [13], and melt penetration and freezing behavior in an instrument tube [14]. Furthermore, great progresses have been made in understanding melt spreading [15, 16] and MCCI [17, 18]. Through these studies, it has been shown that MPS method is capable of accurately analyzing phase changes, melt convection and stratification, and heat transfer, which are the key physical phenomena, governing behavior of the melt spreading and progress of MCCI. This paper summarizes some of the recent findings from these studies.

2. MPS method

2.1. Basic MPS method

The MPS method of Waseda University is based on MPS-SW-MAIN-Ver2.0 developed by S. Koshizuka and K. Shibata [19]. Governing equations are the mass, momentum and energy conservations as described below.

\[
\frac{D\rho}{Dt} = 0 \tag{1}
\]

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

\[
\frac{Dh}{Dt} = k \nabla^2 T + Q \tag{3}
\]

Where, \( \rho \) is density, \( u \) is velocity, \( P \) is pressure, \( \nu \) is kinematic viscosity, \( g \) is gravitational acceleration, \( h \) is enthalpy, \( k \) is thermal conductivity, and \( Q \) is heat source. Equation 1 indicates that the fluid is incompressible. Equation 2 is the Navier–Stokes equation, consisting of the pressure gradient, viscous, surface tension and gravity terms. The right hand side of the energy conservation equation (Eq. 3) consists of heat conduction and heat source terms.

The gradient, divergence and Laplacian operators in the above governing equations are expressed with the particle interaction model as follows.

\[
(\nabla \phi)_i = \frac{d}{dn} \sum_{j=1}^{n} \left( \frac{\phi_j - \phi_i}{|r_j - r_i|^2} \right) \omega(|r_j - r_i|) \tag{4}
\]

\[
(\nabla \cdot \mathbf{u})_i = \frac{d}{dn} \sum_{j=1}^{n} \left( \frac{(u_j - u_i) \cdot (r_j - r_i)}{|r_j - r_i|^2} \right) \omega(|r_j - r_i|) \tag{5}
\]

\[
(\nabla^2 \phi)_i = \frac{2d}{\lambda n^5} \sum_{j=1}^{n} [(\phi_j - \phi_i) \omega(|r_j - r_i|)] \tag{6}
\]
Where, \( \lambda = \frac{\sum w_j |r_j - r| |r_j - r_i|^2}{\sum w_j |r_j - r_i|^2} \) = \( \int_0^\infty \sum w(r) r^2 dv \), \( d \) is number of dimension in the analysis, \( n^0 \) is the initial particle number density, \( r \) is the distance between particles, \( \omega(r) \) is a weight function that determines interactions of neighboring particles by the following equation.

\[
\omega(r) = \begin{cases} 
\frac{r_e - r}{r_e} & (0 \leq r < r_e) \\
0 & (r_e \leq r)
\end{cases}
\]  

(7)

In MPS method, a semi-implicit algorithm is employed. The viscosity term and gravity term from Eq.2 and the temperature are explicitly calculated, while the pressure gradient term is implicitly calculated. In each time step, the momentum equation is first explicitly solved to obtain temporal velocities and positions except the pressure gradient term. Then the pressure is calculated implicitly with the following Poisson equation of pressure (Eq. 8) deduced from the mass conservation equation to maintain the incompressibility of the fluid. Then the positions and velocities of the particles are corrected by the pressure gradient as shown in Eqs. 9 and 10.

\[
\left\langle \nabla^2 P \right\rangle^{k+1} = -\frac{\rho^0}{\Delta t^2} \frac{n^* - n^0}{n^0} 
\]

(8)

\[
u^{k+1} = u^* - \frac{\Delta t}{\rho^0} \nabla P 
\]

(9)

\[r^{k+1} = r^* - \frac{\Delta t^2}{\rho^0} \nabla P 
\]

(10)

2.2. MPS models for simulating melt behavior and MCCI

In order to analyze melt behavior and MCCI with MPS method, various models have been incorporated and developed and validated, where necessary. In the followings, heat transfer and convection model, and phase change model are briefly described as they are fundamentally important for analyzing melt behavior and MCCI. Details of these models as well as descriptions of other models can be found in the earlier works [12-18].

2.2.1. Heat transfer, radiation and convection models. In order to simulate melting and solidification, heat transfer and temperature calculations are essential. By applying the Laplacian model (Eq. 6), the energy conservation equation (Eq. 3) can be discretized to the following form.

\[
h_i^{k+1} = h_i^k + k \Delta t \cdot \frac{2d}{n_{ij}^0} \sum_j (T_j^k - T_i^k) \omega(|r_j - r_i|) + q_i \Delta t
\]

(11)

Where, \( T \) is temperature. Heat conductivity \( k \) between two particles \( i \) and \( j \) is evaluated as harmonic average of the two particles. Validation of this model can be found in the earlier work [15].

\[
k_{ij} = \frac{2k_i k_j}{k_i + k_j}
\]

(12)

Loss of heat by radiation becomes significant at high temperature. In the developed MPS method, radiation heat transfer is simply modeled as heat removal from free surface particles based on Stefan-Boltzman’s law. Hence, change in temperature of a particle \( i \) is expressed as follows [16].

\[
\Delta T_i = \frac{\varepsilon \sigma A T_i^4}{\rho C_p l_0} \Delta t
\]

(13)

Where \( \varepsilon \) is the emissivity of radiation, \( \sigma \) is the Stefan-Boltzman’s constant, \( A \) is the surface area of particle \( i \) and \( l_0 \) is the initial distance between particles.

In MPS method, density of the particles is assumed to be constant (incompressible fluid). Hence, buoyancy due to variations in temperature is evaluated using Boussinesq approximation.
\[
\frac{Du}{Dt} = -\frac{1}{\rho} \nabla P + \nabla^2 u + g\beta_0 (T - T_0)
\]

Where, \(\beta_0\) is coefficient of thermal expansion. Validation of stratification due to density differences and temperature distribution, taking into account of the above convection model, can be found in the earlier work [13]. Hence, convection due to temperature distribution as well as density differences between different particles (materials) can be simulated by motions of the particles without relying on empirical correlations. Convection of the melt is particularly important when simulating MCCI as it influences temperature distribution of the melt.

2.2.2. Phase change and viscosity models.

Modeling of phase changes is another key aspect of simulating melt spreading and MCCI as crust formation (solidification) and concrete ablation (liquefaction) characterize the phenomena. In MPS method, phase changes are expressed by changes to the state of the particles according to their enthalpy (temperature) and solid fraction (\(\gamma\)). Temperature (calculated as a function of enthalpy) and solid fraction of the particle are calculated as follows.

\[
T = \begin{cases} 
T_s + \frac{h - h_{i0}}{\rho C_{ps}} & h < h_{i0} \\
T_s + \frac{T_l - T_s}{h_{l1} - h_{i0}} (h - h_{i0}) & h_{i0} \leq h \leq h_{l1} \\
T_l + \frac{h - h_{l1}}{\rho C_{pl}} & h_{l1} < h
\end{cases}
\]

(15)

\[
\gamma = \begin{cases} 
\frac{1}{h_{i1} - h_{i0}} & h < h_{i0} \\
1 & h_{i0} \leq h \leq h_{l1} \\
0 & h_{l1} < h
\end{cases}
\]

(16)

When \(\gamma = 0\), the particle is in a completely fluid state; when \(\gamma = 1\), the particle is in a completely solid state; when \(0 < \gamma < 1\), the particle is in a partially fluid and partially solid state. Analysis of melt spreading experiments for stainless steel SPREAD suggested that about 55% of heat of fusion needs to be removed from the melt (i.e. containing 55% solid fraction) to stop the spreading process [20]. This indicated that a critical value of solid fraction to determine when molten materials change from the fluid to solid is important. Validation of the above phase change model is given in the earlier work [15].

Evaluation of viscosity of melt is important when simulating behavior of the melt between the solidus and liquidus temperatures. In MPS method, when it is available, a temperature dependent model is used [17]. In other cases, empirical correlations, such as Ramaccotti’s correlation [21] given below, which depend on the solid fraction is used [14, 16].

\[
v(T) = v_L \exp \left( 2.5 C \gamma \right)
\]

(17)

Where \(v_L\) is the kinematic viscosity in liquid phase, \(C\) is a constant, which are experimentally determined (generally ranging between 4 and 8).

3. MPS simulations of melt spreading and MCCI

3.1. Melt spreading analyses

In order to investigate capability and issues of the MPS method to simulate melt spreading and solidification behavior, FARO L26S experiment [22] was analyzed. In the experiment, mixture of UO₂
and ZrO₂ (mass fraction 80:20) was used as simulated core melt and was poured to stainless steel floor via vertical tube. The corresponding MPS simulation geometry is depicted in Fig. 1. The particle size is 2.0 cm and 2496 particles are used to represent the incoming melt. More details of the analysis condition can be found in the reference [16]. One of the key features of this spreading experiment was high viscosity of the melt due to small superheat (initial melt temperature was 2950 K) relative to liquidus temperature (2910 K) and solidus temperature (2860 K) of the melt. Another feature was the small difference between the liquidus and solidus temperatures, which led to significant crust formation during spreading.

Figure 2 shows MPS simulation result of FARO experiment. As the melt spreads, it loses its enthalpy by radiation as described by Equ. 13 and also by heat conduction to the floor as described by Equ.11. Hence, the melt solidifies (crust is formed) as it loses its enthalpy as described in Equ. 15. Hence, viscosity of the melt increases exponentially as it loses its enthalpy (as its solid fraction is increased) as described by Equs. 16 and 17. When solid fraction of a particle reaches 1.0, the particle type is transformed from liquid to solid (crust). The crust hinders spreading of the melt until it is re-melted, or the melt coming from behind flows over the crust. In order to simulate such highly viscous flow with a manageable time step, implicit technique for calculating the viscous term was adopted [16].

Figure 3 shows comparison of time history of leading edge of the melt evaluated by the MPS method and measurements from the experiment. Result obtained by MELTSPREAD code is also shown for comparison [23]. The stepwise spreading propagation is an important feature of highly viscous melt spreading with low superheat. Unlike the result of MELTSPREAD, MPS method reproduced the stepwise profile of the front edge due to crust formation and re-melting of the spreading front, although there are some differences in the timings. Stopping of spreading by crust formation may become more significant when cooling of the melt is considered.
Figure 3. Spreading leading edge of FARO experiment

Spreading simulations by the MPS method have been compared against other experiments. ECOKATS-V1 was one of the ECOSTAR project experiments which utilized oxide mixture melt [24]. The oxide melt was composed of Al₂O₃ (41%), FeO (24%), CaO (19%) and SiO₂ (16%) and was flowed down to a liner ceramic floor. SPREAD tests involved spreading of stainless steel melts in test sections that mimicked the key features of the GE BWR Mark I containment [25]. The melt was poured into a cylindrical cavity that represented the reactor pedestal. The melt then spread into a large open region simulating the cavity annulus through a doorway. The water spreading test by Theofanous [26] simulated water spreading in a pedestal floor of BWR Mark I containment in 1/10 scale.

Comparisons of MPS simulation results and the measurements for ECOKATS-V1, SPREAD, and Theofanous experiments are shown in Figs. 4, 5, and 6, respectively. For comparison, simulation result by MELTSPREAD code is also shown in Fig. 4. For SPREAD test, only the final spreading area has been measured and is shown in Fig. 5 as a constant with respect to time. For comparison, simulated results by Debris Spreading Analysis (DSA) module in the SAMPSON code [26] is also shown in Fig. 5.

Unlike FARO experiments, melts in these experiments exhibited low viscosities due to high superheat and showed rather smooth profiles of spreading. Generally, MPS analysis results (and other codes) showed reasonable agreements with the measurements for such low viscous flows. The underestimation for the Theofanous experiment (Fig. 6) may be due to the particle size (resolution) of the simulation. For low viscous flow spreading, the final spreading thickness can be estimated by assuming balance of the surface tension and gravity, giving the final thickness by the following equation.

\[ h_{\text{min}} = \frac{2\sigma}{\rho g} \] (18)
Where, \( \sigma \) is surface tension, \( \rho \) is density, \( g \) is gravity acceleration, and \( e_{\text{min}} \) is the minimum (final) thickness of the spreading fluid. According to this equation, the minimum thickness is about 3.85 mm, which is smaller than the MPS particle size used in the simulation (5.00 mm). Hence, this may be the reason for the underestimation of the spreading area as shown in Fig. 6. In order to investigate this point, surface tension model needs to be implemented in the current study with smaller particle size (smaller than the minimum thickness) and sensitivity study with different particle sizes is needed.

![Figure 6. Spreading area of Theofanous experiment](image)

### 3.2. MCCI analyses

In parallel to the MPS method development and validation for melt spreading, extensive development and validations have been carried out with MCCI experiments such as simulations of the SURC experiments (SURC-2 and SURC-4) [17] and simulations of the SWISS experiments (SWISS-1 and SWISS-2) [18]. These works concentrated on one-dimensional MCCI behaviors, such as ablation process of concrete, including effect of chemical oxidation process (heat) and overlying water pool in the cavity (top flooding). The works are currently being developed to multi-dimensional analyses. Major outcomes from these research works are summarized below. More details can be found in the references [17, 18].

SURC-2 experiment used prototypic UO\(_2\)-ZrO\(_2\) materials of high temperature as melt materials to interact with basaltic concrete, while SURC-4 experiment used 304 stainless steel melt with Zr addition to investigate influence of Zr oxidation on the interaction process [27, 28]. Both tests employed similar experimental apparatus as shown in Fig. 7. The primary test section was an interaction crucible comprised of a 40 cm diameter basaltic concrete slug surrounded by an MgO annulus. The MgO crucible was 100.0 cm high with an outer diameter of 60 cm and an inner diameter of 40 cm. The interaction crucible was instrumented with numerous thermocouple arrays cast into the concrete cylinder and MgO annulus to provide temperature measures during the tests. An induction coil was placed around the crucible to heat and melt the charge within the test article and to sustain the interaction for the duration of the experiment. For both tests, after an initial preheat phase, the charge materials became molten and began to attack the underlying concrete basemat.

The representative moments, simulated by the MPS method for SURC-2 and SURC-4 are shown in Fig. 8. In both simulations, the concrete basemat is gradually ablated by the melt pool and the molten concrete rose and floated in the upper part of the melt pool due to its smaller density compared with that of the melt. Notable difference is with regard to formation of crust (solidified melt) at the interface of the melt pool and the basemat, due to the difference in solidus temperatures of the melts. The prototypic UO\(_2\)-ZrO\(_2\) melt used in SURC-2 had high solidus temperature (2173 K) while that of the stainless steel used in SURC-4 was relatively low (1673 K). Hence, crust was more easily formed in SURC-2 than in SURC-4. Since crust particles do not form convection, heat transfer from the melt to the basemat is significantly reduced when crust layer is formed in the interface, preventing direct
contact of the hot melt and the basemat and slows down the ablation rate. These simulated results are also consistent with the observations in the experiments.

\[
\begin{align*}
\text{Zr} + 2\text{H}_2\text{O} & = \text{ZrO}_2 + 2\text{H}_2 + 701 \text{ kJ/mol Zr} \\
\text{Zr} + 2\text{SiO}_2 & = \text{ZrO}_2 + 2\text{Si} + 190 \text{ kJ/mol Zr} \\
\text{Si} + 2\text{H}_2\text{O} & = \text{SiO}_2 + 2\text{H}_2 + 500 \text{ kJ/mol Si} \\
\text{Si} + 2\text{CO}_2 & = \text{SiO}_2 + 2\text{CO} + 424 \text{ kJ/mol Si}
\end{align*}
\]
In most MCCI experiments, concrete ablations are terminated by switching off heating of the melt. In reality, cooling of the melt may be required to terminate MCCI by removing the decay heat. SWISS-1 and SWISS-2 experiments were conducted to investigate interactions of 44 kg of 304 stainless steel with limestone/common sand concrete in the presence of an overlying water pool [30]. Stainless steel melt with initial temperature of about 1810 K was delivered to the interaction crucible made of MgO ceramics. Both SWISS experiments were similar in every respect with the only difference being the timing of water addition (at 1914 sec for SWISS-1 and at 99 sec for SWISS-2). Hence, analyses by the MPS method were carried out for SWISS-1 and SWISS-2 to investigate capability and issues of the method to simulate effect of overlying water on MCCI.

The representative moments, simulated by the MPS method for SWISS-1 and SWISS-2 are shown in Fig. 10. The two simulation results are compared until the start of water injection of SWISS-1 to investigate the effect of overlying water pool. For SWISS-2, nucleate boiling heat transfer is considered on the interface between the melt and the water pool. The heat flux is estimated by the following empirical correlation as adopted by other researchers [31].

$$q'' = 8.7 \times 10^6 \Delta T_{sat}^{3/2} [W/m^2]$$  \hspace{1cm} (23)

Where $\Delta T_{sat}$ is the superheat of the melt (or crust) surface. The heat removed by nucleate boiling from the top surface of the melt (or crust) is evaluated by the above equation, but is also limited by the critical heat flux, which is $4.7 \times 10^6 [W/m^2]$ when subcooling of the water is 45 K (SWISS). Transition and film boiling are not considered, but radiation heat transfer is considered. As the result, distinct difference can be seen between the two simulations, namely the crust formation on top of the melt pool with top flooding (SWISS-2).

Both in the experiment and simulation, the crust was supported by the sidewall and small cavity was created between the melt pool and the crust, which prevented effective cooling of the melt. Hence, water injection in SWISS experiments did not terminate MCCI ablation process, though the ablation rate was slightly reduced. As indicated in Fig. 11, calculated ablation front by the MPS method agreed well with the measurements for both SWISS-1 and SWISS-2. However, the MPS simulation underestimates heat flux to the water pool as shown in Fig. 12. This may be due to neglecting water ingressation (penetration of water through the crust) in the simulation. More study is also needed to investigate effects of crust breach and melt eruption on cooling of the melt and termination of MCCI.
4. Conclusions

The MPS method has been extensively studied and developed for simulations of different phenomena involved in severe accident of nuclear reactors at Waseda University. In particular, the developed MPS methods have been successful to simulate melt behavior such as spreading (including behavior of highly viscous melt) and MCCI (including influence of overlying water pool), which are key phenomena in the late phase of severe accidents. Through these studies, importance of modeling phase changes, convection and stratification of the melt and heat transfer have been clarified. Further studies are needed regarding modeling of crust formation and breach as well as termination mechanism of MCCI. Multi-dimensional analyses are needed to investigate anisotropic ablation during MCCI.
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