Numerical simulation of solidification phenomena of single molten droplet on flat plate using E-MPS method

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Received: 13 May 2018; Accepted: 8 July 2018

Abstract
When sand particles and volcanic ash are ingested into jet engines, they become molten droplets and are solidified on the surfaces of the turbine blades and endwalls. This is called the deposition phenomenon, and it causes serious problems in the aircraft, e.g., deterioration of the turbine performance and disturbing the cooling flow of the turbine blade. Therefore, the mechanism of the deposition phenomenon should be clarified in order to predict or prevent engine failure. In the present study, we perform three-dimensional numerical simulations of the deposition behavior of a single molten droplet on a cooled substrate using an explicit-moving particle simulation method. The results show a reasonable agreement with the experimental data. We confirm the formation of finger-like-structures that have the characteristic shape of a droplet that has adhered to an edge, and we also investigate effects of the impact angle on the deposition phenomenon.

Keywords : Deposition phenomenon, Molten droplet, Heat transfer, Explicit-moving particle simulation

1. Introduction
When jet engines are operated in volcanic ash clouds or sandy ground, sand or ash is ingested and melted in a high-temperature combustion chamber. Because turbine components (e.g., blades, cooling flow orifices, endwalls, etc.) are colder than molten droplets, some droplets adhere to and accrete on these surfaces. The deposition phenomenon not only leads to the deterioration of the turbine performance (e.g., blade performance and cooling effect) but also increases its maintenance cost. Therefore, the understanding and prediction of the deposition phenomenon are of significant importance.

The effect of the deposition phenomenon in a gas turbine has been investigated numerically and experimentally. Kim et al. (1993) conducted an experimental study of the deposition phenomena of volcanic ash in an actual engine. They showed that the block of the cooling holes by the ash deposition since the distribution of the deposition is strongly influenced by whether the particles are able to follow the flow. Sundaram and Thole (2006) investigated the influence of the deposition phenomenon on a vane endwall film cooling. Wakikuromaru et al. (2012) reproduced the deposition phenomenon in the case of film cooling turbine blades by means of numerical simulations in order to build a sticking probability model that depends on the wall temperature and particle collision speed. Webb et al. (2012) conducted an experimental study on coal ash deposition. They evaluated and quantified the thickness of sediments for four different ash types and showed that the chemical properties of the ash also played a crucial role in the deposition formation and its thickness. Barker et al. (2012) numerically investigated the coal ash deposition in a high-pressure turbine vane passage.
Singh and Tafti (2016) conducted numerical simulations of deposition phenomena in a two-pass internal cooling duct. As mentioned above, several experiments and numerical simulations have been performed with respect to deposition phenomena. However, the modeling of the deposition phenomenon has not been established yet. In order to prepare an accurate model for simulating the deposition phenomenon, the solidification process of a single droplet is expected to provide some physical insights.

The deposition phenomenon of a single molten droplet has been investigated for application in spray-coating technology. Aziz and Chandra (2000) experimentally investigated the collision and solidification of a single molten droplet. They also studied the finger-shape formation of the adhered droplet and developed a theoretical formula to obtain the number of fingers that form. Accordingly, Shakeri and Chandra (2002) and Mehdizadeh et al. (2004) investigated the effects of the surface roughness and surface temperature on the deposition phenomenon, respectively. Furthermore, Tabbara and Gu (2012) presented numerical simulations of accelerated molten metallic droplets using a volume of fluid method. They clarified the break-up phenomenon at impact and the variation in the solidification process for various impact velocities.

In the present study, in contrast to the volume of fluid method, a moving particle semi-implicit method (Koshizuka and Oka, 1996) is employed to simulate the deposition process of a single molten droplet. The moving particle semi-implicit method (referred to as the MPS method, hereafter) was originally developed for incompressible fluid simulations. As the physical quantities are defined as discretized elements, it is easy to use this method to simulate a free surface in multiphase flows. Therefore, the MPS method is extended to various multiphase flow simulations (Ikeda et al., 1998; Gotoh et al., 2001; Ikari et al., 2006; Kawaguchi et al., 2012; Takahashi et al., 2016). Nakamoto and Yamamoto (2015) performed numerical simulations of the collision and solidification process of a single molten droplet on a flat plate using the MPS method. In order to simplify the simulation, the simulations were conducted in two dimensions without considering the latent heat transfer during the transition phase of the solidification. However, the actual deposition phenomenon apparently occurs in three dimensions, and the latent heat plays an important role in the solidification process.

In this paper, therefore, we conduct three-dimensional simulations of the deposition behavior of a single molten droplet on a flat surface using the MPS method while taking into consideration the latent heat during the solidification process. The obtained results are compared with the existing experimental data (Shakeri and Chandra, 2002), and we discuss the influence of the impact angle on the deposition behavior. This paper is structured as follows: in section 2, the details of the computational conditions are summarized; in section 3, we present the simulation results and discussion; in section 4, we present our conclusions.

2. Numerical simulation

In this study, we perform numerical simulations of a single molten droplet that collides with and adheres to a flat cooled plate. Figure 1 shows the initial condition of the single molten droplet. The numerical condition is set such that it is similar to that of the experiments conducted by Shakeri and Chandra (2002): the droplet consists of Sn; the collision angle is 90 degrees (i.e., the droplet collides normal to the substrate); the initial diameter of the droplet $D_0$ is set as 2.2 mm; the initial temperature of the droplet is 519K; the initial speed of the droplet is $v_0 = 4.0 m/s$; the substrate is fabricated from stainless steel; and the substrate temperature is maintained constant at $T_{wall} = 298 K$. The physical properties of Sn are summarized in Table 1. We select Sn as the material of the droplet although sand and ash are a major factor of the deposition phenomenon in an actual gas turbine. This is because there is experimental data presented by Shakeri and Chandra (2002) that is available for validating the numerical data. In addition, not only the 90-degree case, but also the

![Fig. 1 Collision of the molten droplet with substrate.](image-url)
30-, 45-, and 60-degree cases are investigated in section 3.2.

The numerical simulation is conducted using the explicit-MPS method (referred to as the E-MPS method, hereafter) presented by Oochi et al. (2010). In the E-MPS method, the pressure is solved explicitly to reduce the computational cost. The molten droplet is represented by an aggregation of the computational particles having a very small diameter. The number of computational particles is approximately 195,000. All the computational particles are in the liquid state initially. The governing equations are the continuity, Navier–Stokes, and energy equations, which can respectively be expressed as

\[
\frac{D\rho}{Dt} + \rho \nabla \mathbf{u} = 0, \tag{1}
\]

\[
\frac{D\mathbf{u}}{Dt} = -\frac{1}{\rho} \nabla P + \nu \nabla^2 \mathbf{u} + g + \frac{1}{\rho} \sigma \kappa \mathbf{n}, \tag{2}
\]

\[
\frac{DT}{Dt} = \frac{k}{\rho C_p} \nabla^2 T + \frac{1}{\rho C_p} Q, \tag{3}
\]

Here, \( \mathbf{u} \) is the velocity vector, \( \rho \) is the density, \( P \) is the pressure, \( \nu \) is the kinematic viscosity, \( g \) is the acceleration of gravity, \( \sigma \) is the surface tension coefficient, \( \kappa \) is the curvature, \( \delta \) is the delta function, \( t \) is the time, and \( \mathbf{n} \) is the normal vector of the free surface. For the energy equation, \( T \) is the temperature, \( C_p \) is the specific heat, \( k \) is the thermal conductivity, and \( Q \) is the amount of heat generation. We imposed a no-slip condition on the substrate. When the molten droplet approaches the substrate and the distance from the surface becomes less than the influence radius assumed in the E-MPS method, the heat transfer between the droplet and substrate begins.

In the E-MPS method, these equations are spatially discretized by using the gradient and Laplacian models as follows:

\[
\nabla \phi_i = \frac{d}{dt} \sum_{j \neq i} \frac{\phi_j - \phi_i}{|\mathbf{r}_{ij}|} \mathbf{r}_{ij} w_{ij} (r_{ij}), \quad \nabla^2 \phi_i = \frac{2d}{\lambda n_0} \sum_{j \neq i} (\phi_j - \phi_i) w_{ij} (r_{ij}). \tag{4}
\]

Here, \( \phi \) is a physical quantity such as velocity, \( d \) is the dimensional number of calculation, \( n_0 \) is the number of density of the particles, and \( w_{ij} \) is a weight function. The subscripts \( i \) and \( j \) are indices of the computational particles and \( \mathbf{r}_{ij} \) is a distance vector between the \( i \)-th and \( j \)-th particles. The coefficient \( \lambda \) is defined as

\[
\lambda = \frac{\sum_{j \neq i} |\mathbf{r}_{ij}|^2 w(|\mathbf{r}_{ij}|)}{\sum_{j \neq i} w(|\mathbf{r}_{ij}|)}, \tag{5}
\]

where \( w \) is a weight function.

Subsequently, the discretization of the energy equation is explained. If the computational particle \( i \) is affected by either the surrounding coagulated particles or melted particles, the temperature of the computational particle \( i \) can be expressed as

\[
T_i^{n+1} = T_i^n + \frac{k_i}{\rho_i C_p i} \Delta t \frac{2d}{\lambda n_0} \sum_j (T_j^n - T_j^n), \tag{6}
\]

where \( \Delta t \) is a time step size, and the superscript \( n \) indicates the time step. Furthermore, if the particle \( i \) is affected by both the surrounding coagulated particles and melted particles \( j \), the following discretization is used:

\[
T_i^{n+1} = T_i^n + \frac{k_i}{\rho_i C_p i} \Delta t \frac{2d}{\lambda n_0} \sum_j \frac{1}{2} (T_j^n - T_j^n), \quad T_j = \sqrt{\frac{\rho_j C_j k_j T_j^n}{\rho_j C_j k_j}} + \sqrt{\frac{\rho_j C_j k_j T_j^n}{\rho_j C_j k_j}}, \tag{7}
\]

where \( T_s \) denotes the mean temperature of the particles \( i \) and \( j \). It should be noted that the surrounding particles can be in the solid or liquid phase.

Table 1 Physical properties of Sn.

| Property            | Value          |
|---------------------|----------------|
| Thermal conductivity| \( k_{\text{liquid}} = 33.6 \text{W/mK} \)
|                     | \( k_{\text{solid}} = 62.2 \text{W/mK} \) |
| Specific heat       | \( C_{p,\text{liquid}} = 2441 \text{/(kg \cdot K)} \)
|                     | \( C_{p,\text{solid}} = 2261 \text{/(kg \cdot K)} \) |
| Density             | \( \rho_{\text{liquid}} = 33.6 \text{kg/m}^3 \)
|                     | \( \rho_{\text{solid}} = 62.2 \text{kg/m}^3 \) |
| Melting temperature | \( T_{\text{melting}} = 505 \text{K} \) |
The latent heat $h_l$ plays an important role in the deposition phenomenon, and the corresponding model is explained below. A schematic of the phase change due to the heat exchange is shown in Fig. 2. When the temperature of the computational particle in the liquid phase $T_l$ reaches the melting temperature $T_{\text{melting}}$, the computational particle is treated as a particle that is in the transient state, and its temperature remains constant at $T_{\text{melting}}$. For the transient particle, the heat loss for each time step $\Delta h$ is computed using the heat conduction equation. If particles $i$ and $j$ are not in the transient phase, $\Delta h$ is computed using

$$\Delta h = \frac{\Delta t}{\rho_i \cdot \Delta t_i} \sum_{j \neq i} \left( k_{ij} (T_j - T_i) \right) w_{ij}.$$  

(8)

If the particles are in different phases, $\Delta h$ is computed with $T_s$ as

$$\Delta h = \frac{\Delta t}{\rho_i \cdot \Delta t_i} \sum_{j \neq i} \frac{1}{2} \left( k_{ij} (T_s - T_i) \right) w_{ij}.$$  

(9)

The mean thermal conductivity $k_{ij}$ is calculated as follows. If the particles $i$ and $j$ are not in the transient phase, we use

$$k_{ij} = \frac{2 k_i k_j}{k_i + k_j}.$$  

(10)

If particle $i$ is in a transient phase, we use the thermal conductivity of the particle $j$; if particle $j$ is in a transient phase, we use the thermal conductivity of the particle $i$ as the thermal conductivity $k_{ij}$. When the computational particle loses all its latent heat $h_l$, the computational particle is treated as a solid-phase particle.

3. Results and discussion

3.1. Collision toward horizontal substrate

In this subsection, the obtained results of the droplet collision on the horizontal substrate are discussed. The numerical condition is set in accordance with the experiment as shown in Fig. 1. The initial velocity of the droplet is set as $v_0 = 4.0 \text{ m/s}$; the collision angle is 90 degrees.

Figure 3 shows a time series of snapshots of the colliding and adhering droplet. The time $t$ begins when the droplet starts falling. The liquid, transient (i.e., liquid to solid), and solid particles are indicated by the red, white, and blue colors, respectively. As shown in Fig. 3(a–c), all the computational particles are in the liquid phase and the droplet begins to drop, collides, and spreads on the surface. At $t = 0.37 \text{ ms}$, void structures are observed in the region around the edge, and these are the origin of the finger-like structure. In this time instant, the liquid particles facing the substrate begin to become cooled owing to the heat transfer from the droplet into the substrate. At $t = 0.5 \text{ ms}$, the droplet spreads substantially and finger-like structures clearly appear around the edge of the droplet. At $t = 1.0 \text{ ms}$, the transient particles are found in a region close to a fringe of the adhered droplet. The transient and solidification are found to be propagated inward the droplet from $t = 1.25 \text{ ms}$ to $t = 2.0 \text{ ms}$ whereas the liquid particles remain in the swelling structure at the periphery. As time advances (Fig. 3(j–l)), the remaining liquid particles begin to solidify.

Figure 4 shows the side view of the droplet solidification. The colliding droplet spreads on the substrate, and the solidification begins from the particles facing the substrate. The droplet spreads substantially at $t = 0.75 \text{ ms}$, and the liquid particles create a swelling structure at the edge of the spreading droplet. As shown in Fig. 4(c–e), the region slightly inside the outer edge first solidifies, then the center region solidifies, and finally the swelling structure solidifies. This is because the time scale of heat conduction varies owing to the thickness distribution. The swelling structure moves inward owing to the surface tension of the droplet. All the computational particles are perfectly solidified at $t = 4.0 \text{ ms}$. A slight undulation is observed on the surface of the perfectly solidified droplet.
Fig. 3  Time series of snapshots of deposition of Sn droplet in case of collision angle of 90 degrees at collision velocity of 4 m/s (bird’s eye view): (a) \( t = 0\) ms; (b) \( t = 0.12\) ms; (c) \( t = 0.25\) ms; (d) \( t = 0.37\) ms; (e) \( t = 0.5\) ms; (f) \( t = 1.0\) ms; (g) \( t = 1.25\) ms; (h) \( t = 1.50\) ms; (i) \( t = 2.00\) ms; (j) \( t = 2.50\) ms; (k) \( t = 3.50\) ms; and (l) \( t = 4.00\) ms.

Fig. 4  Time series of snapshots of deposition of Sn droplet in case of collision angle of 90 degrees at collision velocity of 4 m/s: (a) \( t = 0.37\) ms; (b) \( t = 0.75\) ms; (c) \( t = 1.25\) ms; (d) \( t = 2.00\) ms; (e) \( t = 3.00\) ms; and (f) \( t = 4.00\) ms.
Fig. 5  Time variation of non-dimensional droplet diameter.

Tabbara and Gu (2012) performed a numerical simulation of a Sn droplet under the same conditions as the present study. They employed the volume of fluid method. They observed that a thin solid layer forms on the substrate at the very early stage, and this layer builds up unevenly. As their simulation considers the gas phase around the droplet, the Kelvin–Helmholts instability caused by the shear stress appears at the interface between the liquid and gas phases. The surface of the perfectly solidified droplet then undulates. In contrast with the results obtained by Tabbara and Gu (2012), we observed a thin solid layer on the substrate at a very early stage and its build-up. However, the undulation of the surface of the solidified droplet is not observed as the gas phase around the droplet is not considered.

Figure 5 shows the time variation of the droplet diameter normalized by that after the solidification. The numerical result compares well with the experimental data obtained by Shakeri and Chandra (2002). Here, the time origin $t = 0$ ms corresponds with the time at which the droplet begins to fall. In the present simulation, the droplet diameter rapidly increases after the collision as the adhered area enlarges owing to the collision. The spread speed of the diameter then slows down, which corresponds to the stretching of the edge of the droplet owing to the inertia and the formation of finger-like structures. Subsequently, the diameter decreases slightly owing to an inward movement caused by the surface tension. Finally, the non-dimensional diameter reaches a steady state, and the resultant diameter is approximately three times that of the initial diameter. This time trace of the normalized diameter is qualitatively similar to that in the experiment. However, the resultant diameter is approximately 14 % smaller than that obtained by Shakeri and Chandra (2002): in the present simulation, $D/D_0 \approx 3.0$; and in Shakeri and Chandra (2002), $D/D_0 \approx 3.5$. One possible reason for this difference is the thermal boundary condition: a constant temperature is imposed on the surface of the substrate in the present study; the heat transfer toward the wall is larger than that in the experiment, and this overestimation of the heat transfer to the substrate results in a smaller diameter than that observed in the experiment.

3.2. Collision toward inclined substrate

Subsequently, we performed simulations for three different collision angles. Figure 6 shows the bird’s eye view of the solidifying molten droplet for the colliding angle of 45 degrees. The initial velocity of the droplet is set as $v_0 = 4.0$ ms. The arrow indicates the colliding direction of the droplet, and the substrate is inclined. In the case of the colliding angle of 45 degrees, the droplet spreads on the substrate at $t = 0.5$ ms, and a swell-like structure is formed around the circumference. At $t = 1.0$ ms, the collided and melted droplet moves in the collision direction while solidification begins to occur in the backward region. At this time instant, the near-wall computational particles have already solidified, and the liquid particles move over the solidified computational particles in the collision direction. At $t = 2.4$ ms, the solidification propagates in the collision direction, and the front region is still molten. At $t = 5.1$ ms, the melted particles gather at the tip of the front.

Fig. 6  Solidification of Sn droplet on inclined flat plate. Time is $t = 0.5$ [ms], $t = 1.0$ ms, $t = 2.4$ ms, and $t = 5.1$ ms from left column to right column. Impact angle is 45 degrees.
Fig. 7 Solidification of Sn droplet on inclined flat plate. Time is $t = 0.5$ms, $t = 1.0$ms, $t = 2.4$ms, and $t = 5.1$ms from left column to right column. Impact angles are (a) 30 degrees and (b) 60 degrees.

Fig. 8 Projected area for various impact angles.

region and create a bump-like structure. Moreover, the finger-like structure that is observed in the case of vertical collision does not appear.

Figure 7 shows the solidification process of the molten droplet for the impact angles of 30 degrees and 60 degrees. In the case of the impact angle of 30 degrees, the solidification behavior is similar to that of 45 degrees. However, the bump-like structure created at the tip is sharper than that obtained at 45 degrees. In contrast, in the case of the impact angles of 60 degrees, a finger-like structure appears around the circumference of the solidified droplet.

The spreading of the droplet is evaluated based on the projected area on the surface of the substrate because the droplet spreads elliptically. Figure 8 shows the time variation of the projected area. In the case of 90 degrees, the projected area rapidly increases and decreases slightly, and the droplet is then perfectly solidified. With the decrease in the impact angle, the projected area gradually increases as compared with the 90-degree case, the time to solidification increases, and the resultant projected area also increases.

4. Conclusion

We performed numerical simulations of the deposition phenomena of a single molten Sn droplet on a flat substrate surface while taking into consideration the latent heat by using the E-MPS method. The cases of four different collision angles are investigated. The results show that the present simulation reproduces the processes of collision, spreading, and coagulation of the droplet on the substrate. In addition, it quantitatively agrees with the experimental data for the collision angle. The time variation of the non-dimensional diameter obtained from the simulation shows a similar tendency to that of the existing experimental results. We also investigated the effects of the impact angle on the deposition behaviors of a colliding droplet. In the cases of the impact angles of 30 and 45 degrees, a finger-like structure does not appear but a bump-like structure is formed at the tip of the droplet; in the case of the impact angle of 60 degrees, a finger-like structure is formed.
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