Simulation of thermal spray process of a three phase flow calculation with substrate temperature of 300K

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Abstract. We propose a particle method (MPS method) which can analyse the large deformation, splitting and coalescence of liquid as a new calculation method and a gas-liquid coupling method of finite volume method which can stably solve the compressible flow. By doing this, we aim to solve the interface resolution problem in the interface capture method and to establish a complicated gas-liquid multiphase flow analysis method that can deal with large deformation case. At the temperature of 300K, the validity of the flow field is consistent with the reference. The processes from the acceleration and deformation of a droplet to the solidification of the droplet on a substrate are successfully being observed. The shape of the splat is influence by substrate temperature.

1. Introduction
Thermal spray is one of the surface treatments that already established many years ago. It is a method that has been used for prevents corrosion, by a film that formed on the base material by using burning flame or electricity that spray the heated molten particles to the material. In the thermal coating process which the molten metal is sprayed, the formation rate of the surface film can be made extremely higher than other surface treatment methods such as plating and vapor deposition. Since the base material has low temperature, the thermal strain is relatively small, and any material can be used as base material such as ceramics, organic material, wood, clothes, and papers, not limited to metals only.

This have been influenced the substances that can be used for thermal spraying. As a result, the thermal spraying method has applied to high performance surface treatment technology such as corrosion prevention and rust prevention, rather than heat resistance, thermal insulation, wear resistance and corrosion resistance. Furthermore, it is now being used in devices that used in harsh environments such as thermal power boilers, aircraft jet engines, and marine diesel engines. Instead of having outstanding characteristics, there is a problem that related to low adhesion efficiency and required the roughening process for the substrate.

Droplets in thermal spray may experience three processes during surface treatment, which are acceleration, solidification and lamination process. Phenomena that can occur with these elementary processes are thought to be different. In the collision flattening solidification process, large deformation is notified mainly due to collision, splitting phenomenon and cooling and also solidification. In the lamination process, stacked droplets coalescence and mechanical interlocking can be observed. In the thermal spraying process, it is difficult to explain the phenomenon by combining these phenomena continuously. Once this droplets contact with the base material (substrate), we called
it splat. Since this elementary process of this splat is a \( \mu \)meter size and very rapid condition (like splash), so it is difficult to observe all this process via experiment, which has been proven by [1][2].

In multiphase flow simulation, an approach called Volume of Fluid (VOF) method is widely used. But this method has difficulties to capture in detail what happened in the interface. This interface is depends on the mesh, and if we want to analysis of droplet particles collide, flying and deformed at the substrate, it is necessary to use the entire domain between the nozzle and the substrate. Consequently, this will take longer computational time and demand very fine domain grid.

The higher speed droplets contact with the substrate to form a coating and flattened due to temperature difference. This flatness was relative to \( \text{Re}^{0.2-0.3} \). CFD analysis on sprayed particles and substrate has been successfully conducted by [1][2]. In this paper, we imposed the Moving Particle Semi Implicit (MPS) coupling together with Finite Volume Method (FVM) to answer the interface analysis problem.

2. Methodology

In this investigation, the Reynold-averaged three-dimensional unsteady Navier–Stokes equation is solved with 3\(^{rd}\) order of MUSCL [4]. The air is assumed to be an ideal gas with SLAU is used for non-viscous flux and Sutherland relation is used for viscosity equation calculation. Van Albada limiter is amended and an explicit 3\(^{rd}\) order Total Variation Diminishing Runge-Kutta method is used for time integration [5][6]. A structured grid with total grid points of 7,820,000 is being used in this calculation.

![Figure 1. Structured grid (7.82x10^6) for this study.](image)

Figure 2 shows the droplet calculation conditions, which consists of 7800 particles. In this study, we simulate the conditions of flame spraying, which is the most common thermal spraying method among the actual thermal spraying methods.

![Figure 2. Initial placements of sprayed droplets.](image)

In flame spraying, the velocity at which the spray droplets collide with the substrate changes depending on the distance between the nozzle and the substrate. Therefore, in the calculation of only the MPS method, the droplet velocity is given with reference to the literature [7]. Specifications of the thermal spray particles and the substrate are summarized in Table 1.
Table 1. Specifications of the thermal spray particles.

| Parameter                                      | Value                   |
|------------------------------------------------|-------------------------|
| Droplet Substance                              | Copper                  |
| Substrate Material                             | SUS304                  |
| Distance between initial MPS particle          | 2.0 μm                  |
| Initial Droplet Diameter, $D$                  | 50.0 μm                 |
| Initial Droplet Velocity, $v$                  | 60 m/s                  |
| Initial Droplet Condition (height), $l$        | 1.0 mm                  |
| Initial Droplet Temperature, $T_D$             | 1700K                   |
| Substrate Temperature, $T_S$                   | 300K                    |
| Droplet Solidification Temperature             | 1357K                   |
| Exit Nozzle Speed                              | 100 m/s                 |
| Exit Nozzle Temperature                        | 273 K                   |
| Exit Nozzle Static Pressure                    | 1.0 atm                 |

For interface, the particle on the free domain must satisfy with equation (1)

$$n^0 < \beta n^*$$  \hspace{1cm} (1)

Here, $n^0$ is the initial particle density, and $n^*$ is the particle number density that is calculated after the explicit integration of the velocity field, while $\beta = 0.95$. In addition, Gotoh ASA conditions are imposed as an auxiliary judgment [8]. For solidification modelling, it has been control by solidification fraction, $\gamma$, which has been determined by enthalpy function:

$$\gamma = \begin{cases} 
1 & (h < h_{s0}) \\
\frac{h_{s1} - h}{h_{s1} - h_{s0}} & (h_{s0} \leq h \leq h_{s1}) \\
0 & (h > h_{s1}) 
\end{cases}$$  \hspace{1cm} (2)

$h_{s0}$ is initial enthalpy while $h_{s1}$ is resultant enthalpy of the melting process. Furthermore, the droplet is in liquid form for $\gamma < 0.5$, and in solid form for $\gamma \geq 0.5$. After a particle is solidified on the substrate, then the particles are considered to be stick at substrate.

3. Results and Discussion

3.1 Validation on physical aspect

![Figure 3](image_url1)  \hspace{1cm} ![Figure 3](image_url2)

*Figure 3.* (a) Streamline of the relative velocity of droplets: $Re = 133$. (b) Streamline around the sphere [13]: $Re = 150$
Figure 3 shows streamlines around a sphere at Re = 150 for which Johnson et al. [9] performed experiments and analysis. Comparing these, the separation position of the flow field obtained in this study is slightly forward, but the symmetrical vortices formed in the wake and the position where the separated streamline reappears are almost the same. Therefore, the flow field formed by the droplets obtained in this study was able to analyze the real phenomenon and confirmed its validity.

3.2 Splat shape change by substrate temperature
We aim to deal with the higher interface domain requirement for bigger scale of deformation by coupling between gas-liquid multiphase flow analyses. Figure 4 shows the speed in term of time history from initial distance \( l \) until collide at the substrate.

As explained before, in order to observe the whole process from the initial droplet condition until contact with the substrate (acceleration, solidification and lamination process), it is necessary to calculate all surface between the nozzle and the substrate. As we can see in Figure 4, droplet started at distance \( l \) has initially first contact with the substrate approximately at \( t = 0.4 \mu \text{s} \), where the speed has been slightly change. The whole process can be simulating less than 3\( \mu \text{s} \) second. Furthermore, the speed continuously to reduce and the droplet started to collide with the substrate. When moderate speed has been dominance for the entire droplets, the process of “flying” particles has been initially being occurred. Nearly at \( t = 3 \mu \text{s} \), most of the droplet has obtain the lamination process while the “flying” particle are maintained at the same speed. The two-dimensional cross-section is used since it will be easier to understand by visualization.

**Figure 4.** Speed history (300K).
The movement of the droplets caused the solid droplets to be strongly cooled from the outer edge of the droplets in the process of collision and cooling of the high temperature droplets on the substrate. At the beginning, when the lower part of the droplet and the substrate come into contact, heat conduction occurs and the temperature is lowered by cooling, and conversely, the surface temperature of the substrate is increased (Figure 5). While the outer edge of the substrate is always cooled by the exchange of heat due to heat conduction with the low surface temperature substrate, the surface temperature of the substrate is high and the temperature gradient is large in the stationary droplet center. The temperature of the liquid is kept high because it cannot be obtained. Thus, a distribution was formed where the temperature increased in the direction from the outer edge to the center.

4. Conclusion
In this study, multi-phase flow analysis was performed by combining the finite volume method using a grid and the particle method using particles in the process of droplet flight and collision in the thermal spraying method. The conclusion can be summarized as below.

1) Droplet particles are strongly cooled and solidified from the outer edge, causing deposition to become a factor in shape determination
2) It was confirmed by analysis that the substrate temperature is an important factor of the flat shape
3) Validity of the flow field by droplets obtained by the proposed coupled method was confirmed

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