The Effects of Thermal Shrinkage on Coating Formation in Thermal Spray Processes: 
A Numerical Approach

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Abstract
In this paper, we performed a numerical study on the effects of thermal shrinkage on the deposition of molten tin droplets on a steel substrate in thermal spray coating process using Volume-of-Fluid (VOF) method. Thermal shrinkage is a phenomenon caused by variation of density during solidification and cooling down of molten metal. The Navier-Stokes equations along with the energy equation including phase change are solved using a 2-D axisymmetric mesh. We used the VOF method, applied to the fixed Eulerian mesh, to track the free surface of the droplet. For solidification, we used an enthalpy-porosity formulation. The simulations performed in this study are accomplished using both a commercial code (FLUENT) and an in-house developed program. The results of these scenarios are presented: the normal impacts of 2.7mm spherical tin droplets at 1m/s and 2m/s, initially at 240°C, onto a 27°C steel substrate. It is seen that when the droplet impacts to the substrate with 1m/s velocity, it spreads and solidifies and during the recoil of the droplet, a single cavity forms within the splat which is the source of porosity and is caused by shrinkage.

Keywords: thermal shrinkage, thermal spray coating, VOF method, solidification, droplets.

1. Introduction
In thermal spraying processes, coatings such as various metals and alloys, carbides, and ceramics are applied to metal surfaces by a spray gun with a stream of oxyfuel flame, electric arc, or plasma arc. These coatings are formed by spraying and deposition of molten droplets on the substrate. The properties and quality of these coatings depend on many factors such as flame/laser/arc, material used for spraying, substrate and spray characteristics.

Another phenomenon that affects the shape of droplets in thermal spraying is thermal shrinkage. Because of their thermal expansion characteristics and changes in density, metals shrink or contract during solidification and cooling. Shrinkage, which causes dimensional changes and sometimes cracking, is the result of:

a) Contraction of a molten metal as it cools prior to its solidification.

b) Contraction of the metal during phase change from liquid to solid (release of the latent heat of fusion).

c) Contraction of the solidified metal (casting) as its temperature drops to the ambient temperature.

The largest amount of shrinkage usually occurs during the third period. In fact, shrinkage occurs because in most of the materials the volume decreases due to an increase in density when the material undergoes solidification and cooling. Shrinkage can cause various defects in manufacturing processes. These defects can affect the appearance or even the structural integrity of the final product. Some examples are cavities, porosities, discontinuities such as cracks, defective surface etc. In a thermal spraying process, shrinkage has some effects on the deposition of droplets on the substrate and the formation of coating including porosity, cavity, curling up of splat and surface depression.

Generally, developing a model to simulate impacts and solidification of molten droplets on to the substrates is a complex problem. This problem involves computing heat transfer and fluid flow in a droplet with a moving free surface which is undergoing phase change, and adding density variation makes the problem more complex.

Modeling droplet impacts has a long history. Harlow and Shannon were the first to simulate the impact of droplets [1]. Later, Tsurutani et al. [2] and Trapaga and Szekely [3] studied the impact of molten droplets in thermal spraying processes. More studies [4-13] were done by Liu et al., Pasandideh-Fard et al., Zhao et al., Fukai et al., Bertagnolli et al., and Waldvogel and Poulikakos. Moreover, Bussmann et al. [14,15] developed a 3D model to simulate water droplet impacts and Pasandideh-Fard et al. [16,17] extended it to study metal droplet impacts. A level set method was also developed by Zheng and Zhang [18] to study droplet impact and phase change with no shrinkage.

To model shrinkage during solidification, Toutant and Argyropoulos [19] developed a numerical model for cylindrical casting of aluminum and magnesium based on a fixed-grid 2D axisymmetric mesh. A similar model was presented by Beech et al. [20,21] to compute solidification shrinkage in cylindrical and T-
shaped castings in Flow-3D software. Also Kim and Ro [22] had a similar study on the occurrence of solidification shrinkage in a 2D rectangular mold. All algorithms mentioned above, are suitable for cases in which the liquid is quiescent and the geometry is simple. Therefore, MacBride et al. [23] presented a 2D model to account for directional solidification in dendritic binary alloys which includes the effect of shrinkage-induced flow. Similarly, Chiang and Tsai [24] analyzed fluid flow and domain change caused by solidification shrinkage in a 2D rectangular cavity filled with molten alloys. Finally, using a 2D finite volume model based on the volume averaging, Ehlen et al. [25] predicted the transient shape of the melt surface, the shrinkage cavity locations, and their influence on the final solute distribution of AlSi alloy. Moreover, to apply the volume-of-fluid (VOF) method to the cases where the density is not constant, they modified the classic donor-acceptor flux approximation. Finally, Raessi et al. [26] modified the model used by Pasandideh-Fard et al. [17] to account for density variation and modeled shrinkage in solidification of metal droplet impacts.

In this paper, numerically we study the effects of shrinkage and density variation in solidification of molten tin droplets while they impact and spread on cold steel substrates. To do this, we used both a commercial code (Fluent) and an in-house developed program. Results of the two setups are compared with the available experiments. In this study, densities of the solid and liquid phases are assumed to be linearly changed with temperature.

2. Numerical Method

2.1. Fluid Flow

In this paper, fluid flow of the impacting droplet is modeled using a finite-difference method. Navier-Stokes equations are solved in both axisymmetric and three dimensional coordinate systems. Liquid which in this case is the molten metal is modeled as an incompressible fluid and since Reynolds number is in the order of 10^5, fluid flow is assumed to be linear. Using the volume of fluid technique (VOF) applied to a fixed Eulerian mesh, the free surface of the droplet is tracked. In this technique, a scalar function f is defined. This function shows the fraction of a cell which is filled with fluid. When a cell is fully occupied by fluid, it is set to unity and consequently when a cell is empty of fluid, f equals to zero. In other cases f is between zero and one. For surface tension we used the continuum surface force (CSF) model integrated with smoothed values of function f in evaluating free surface curvature. Surface tension is assumed to be constant but thermal conduction and especially density are taken to vary with temperature. Further details of fluid flow simulations can be seen elsewhere [15,17]. Properties of tin for droplets, stainless steel for substrate and air are taken from Incropera and DeWitt [27, 28], Raessi et al. [26] and Stankus and Khairelun [29].

2.2. Heat Transfer and Solidification

Enthalpy in the droplet is calculated as the sum of sensible enthalpy h and latent heat $\Delta h$ as follows:

$$H = h + \Delta h$$  

in which

$$h = h_{ref} + \int_{ref}^{T} c_p dT$$  

In this relation, $h_{ref}$ and $T_{ref}$ are the reference enthalpy and temperature, respectively, and $c_p$ is the specific heat at constant pressure.

For solidification, we used an enthalpy-porosity technique in which the liquid-solid front is not tracked explicitly. Instead a quantity named liquid fraction $\beta$ is used in every cell in the form of following relations:

$$\beta = \begin{cases} 0 & \text{if } T < T_{solidus} \\ \frac{T - T_{solidus}}{T_{liquidus} - T_{solidus}} & \text{if } T_{solidus} < T < T_{liquidus} \\ 1 & \text{if } T > T_{liquidus} \end{cases}$$

In fact, liquid fraction shows the fraction of every cell which is filled with liquid material (molten metal). The second term in the previous relation represents a zone in which the liquid fraction is between zero and one. This zone is called the solidification mushy zone and is modeled as a pseudo porous medium. As the material solidifies in a cell, porosity reduces from 1 to zero ($\beta = 0$) and also velocity becomes zero.

By definition of liquid fraction, we can now write the latent heat content in terms of the latent heat of material:

$$\Delta H = \beta L$$

In this relation, L is the latent heat of material and $\Delta H$ can vary between zero for solid and L for liquid. We can now define the energy equation for solidification/melting problems as the relation below:

$$\frac{\partial}{\partial t} (\rho H) + \nabla \cdot (\rho \mathbf{v} H) = \nabla \cdot (k \nabla T) + S$$

where $\rho$ is density, $\mathbf{v}$ is fluid velocity and S is source term.

When Eq. (4) is used directly to update the liquid fraction in iteration for obtaining temperature, it results in poor convergence of the energy equation for pure materials where $T_{Solidus}$ and $T_{Liquidus}$ are equal (like in this paper). Therefore, we used a method based on specific heat, given by Voller and Prakash [30] instead.
As mentioned, the enthalpy-porosity treats the mushy zone as a pseudo porous medium. When $\beta$ reduces during solidification in a cell, velocity drops to zero. The momentum sink due to this reduced porosity, can be shown in the following form:

$$
S = \frac{(1 - \beta)^2}{(\beta^3 + \varepsilon)} A_{mush} (v - v_p)
$$

(6)

where $\varepsilon$ is a small number to prevent division by zero. $v_p$ is the pull velocity which is set to zero here because the solidified material is not pulled out of the domain (like in continuous casting processes). $A_{mush}$ is the mushy zone constant and specifies the slope at which velocity drops to zero, as the material solidifies. Increasing this constant makes the slope steeper.

2.3. Shrinkage

To measure the amount of shrinkage in a material, shrinkage factor is defined as follows:

$$
\text{Shrinkage factor} = \frac{\rho_s - \rho_l}{\rho_l}
$$

(7)

where $\rho_l$ and $\rho_s$ are the densities of liquid and solid phases, respectively. Table 1 shows the amount of shrinkage factor (for solidification) for some metals/alloys.

### Table 1: Shrinkage factor for some metals/alloys [31]

<table>
<thead>
<tr>
<th>Metal/Alloy</th>
<th>Shrinkage Factor (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Aluminum</td>
<td>6.6</td>
</tr>
<tr>
<td>Carbon Steel</td>
<td>2.5 – 3</td>
</tr>
<tr>
<td>White Iron</td>
<td>4 – 5.5</td>
</tr>
<tr>
<td>Tin</td>
<td>3.3</td>
</tr>
</tbody>
</table>

For tin, the density variation with temperature is demonstrated in Fig. 1; the values are taken from Stankus and Khairulin [29]. As shown in Fig. 1, density decreases with increasing temperature.

![Figure 1: Density variation for tin](image)

However, there is a discontinuity in density when material undergoes solidification and changes phase from liquid to solid. This discontinuity caused the solution to diverge. To avoid this problem, we assumed that in the region where the process is taking place, density changes linearly with temperature. We applied density in our simulations as piecewise polynomials.

Tin droplets impact at 240°C and the substrate is initially at 27°C. Using our data for tin densities and the relation for shrinkage factor, its value for the droplet in this process would be 4.42%. This amount involves liquid phase, solidification and solid phase shrinkage.

3. Results and Discussion

Tin properties are listed in Table 2. Like density, thermal conductivity is taken to be linear. Tin droplets impact at a temperature of 240°C onto the stainless steel substrate which is at 27°C. A contact resistance is considered between the droplet and the substrate. This resistance is estimated to be approximately $5 \times 10^{-6}$ m²K/W [9].

Figure 2 shows the results for the 2D axisymmetric analysis. In this study, droplet impacts with a velocity of 1m/s. Before impact, it is assumed that the droplet has the shape of a sphere with a diameter of 2.7mm. As the droplet impacts, it begins to spread on the substrate and since the temperature of the substrate is less than that of the droplet, it solidifies and deposits on the substrate. At (t = 4.5 ms) droplet reaches its maximum spread on the surface since the effects of surface tension forces overcome the effects of inertial forces. At this time, the droplet is like a flattened disk with raised rims and a part of droplet which is in contact with the cold substrate is solidified (t = 4.5 ms). After this time, the effects of surface tension forces cause the remaining molten part of the droplet to recoil on the solidified layer and form a recoiling ring. This ring meets at the center of the droplet and, as a result, a void is formed at the center of the deposited droplet. Close inspection of the numerical results reveals that this void is caused by shrinkage. The recoiled molten tin reaches a maximum height between 8.3ms and 11.3ms (approximately at t=10 ms) elapsed after the impact. Capillary effects cause necking in the molten column. This phenomenon can be seen in the results shown in Fig. 2. Later, the melt column falls down under the effects of gravity and surface tension. Finally, after the entire molten tin is solidified, a splat remains on the substrate.

Figure 2 also shows the calculated temperature distribution in droplets. It is clear from this figure that as the droplet makes its first contact with the substrate, it begins to lose heat through the wall. In this study, the effects of ambient air on the droplet and heat transfer between air and droplet is taken into account. In displaying the figure, however, the temperature distribution inside air is not shown because the droplet domain is of interest in this study.
Table 2: Properties of tin in solid and liquid phases

<table>
<thead>
<tr>
<th>Phase</th>
<th>Density (kg/m$^3$)</th>
<th>Thermal conductivity (W/m K)</th>
<th>Specific Heat (J/kg K)</th>
<th>Kinematic viscosity (m$^2$/s)</th>
<th>Surface tension (N/m)</th>
<th>Latent heat (kJ/kg)</th>
<th>Melting point (°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Solid</td>
<td>1.491T+7733</td>
<td>0.154T+113.0</td>
<td>244</td>
<td>2.7 x 10$^{-7}$</td>
<td>0.526</td>
<td>60.9</td>
<td>232</td>
</tr>
<tr>
<td>Liquid</td>
<td>243</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

Figure 2: Computer generated images of temperature distribution in a 2.7mm dia. tin droplet impacting at 240°C with a velocity of 1 m/s onto a stainless steel substrate initially at 27°C. The left half of each image relates to the case with variable density (i.e. with shrinkage) and the right half belongs to the constant density. Solidified regions are separated from molten regions with a black line.

It can be seen in Fig. 2 that in the peripheral regions of the splat where the thickness is smaller (i.e. the thermal resistance is smaller) the temperature drops faster than in the central regions. Also, shrinkage in these regions reduces the maximum amount of spread on the substrate.

Figure 3 shows the impact of droplets with an initial velocity of 2 m/s. In comparison with Fig. 2 in which the initial velocity was 1 m/s, the droplet spreads more on the surface and the thickness of the deposited droplet is less than in the previous case, this in turn causes the droplet to solidify and cool down much faster. Because of this initial velocity, the droplet does not recoil and, as a result, there would be no void in the center of the final solidified splat in contrast to what is seen for the case of 1 m/s (Fig. 2). This is an advantage and can be used to reduce the effects of shrinkage in forming macroporosities. Although the effects of shrinkage are not clear in the first three images of Fig. 3, the difference between the variable and constant densities can be seen in the last image (t = 21.02 ms) where the droplet is completely solidified. It can be seen that the surface of the droplet is further depressed when shrinkage factor is considered. The image shows that the splat surface for the left half related to the case with variable density is lower than that of the right half with constant density.
4. Conclusion
In this paper, we studied the effects of thermal shrinkage on deposition and formation of porosity in molten tin droplets on a steel substrate. We used a 2-D axisymmetric mesh in which we solved the Navier-Stokes equations and used VOF model to track the free surface of the droplet as it spreads on the substrate. We also accounted for solidification and density variation which leads to thermal shrinkage. We applied the model to two scenarios in which droplets of 1 m/s and 2 m/s with a temperature of 240°C and diameter 2.7mm impact normally to a 27°C steel substrate. In the first case, as the droplet spreads on the substrate and recoils, a small void remains in the center of the solidified splat. This void is caused by shrinkage and as the figures show, it cannot be seen when the density is constant. For the second case, because of a high initial velocity, the droplet spreads more on the substrate and, as a result, there will be no recoiling towards the center of the droplet and no void will be formed. Effects of density variation in this case are less important than the other case. However, the differences between the variable density and constant density can still be recognized.

References


