

SPH based modelling of oxide and oxide film formation in gravity die castings

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Abstract. Gravity die casting is an important casting process which has the capability of making complicated, high-integrity components for *e.g.* the automotive industry. Oxides and oxide films formed during filling affect the cast product quality. The Smoothed particle hydrodynamics (SPH) method is particularly suited to follow complex flows. The SPH method has been used to study filling of a gravity die including the formation and transport of oxides and oxide films for two different filling velocities. A low inlet velocity leads to a higher amount of oxides and oxide films in the casting. The study demonstrates the usefulness of the SPH method for an increased understanding of the effect of different filling procedures on the cast quality.

1. Introduction

Gravity die casting is an important casting process which has the capability of making complicated, high-integrity components for *e.g.* the automotive industry. In gravity die castings, the major defects are porosity and entrapped oxide/oxide films and inclusions, which affect the mechanical strength of the cast product [1]. In addition to the design of the mould and the gating system, the ingate velocities significantly affect the number and distribution of the oxides generated from the filling stage. Improvements to product quality and productivity can be brought about through a better control of the die filling. Numerical simulation offers a powerful and cost effective way to study the effectiveness of different die filling procedures and die designs [2, 3, 4].

During the casting, liquid metal oxidizes only for the time period the metal is exposed to air, i.e., when there is a free surface. The oxides formed are subsequently transported by the melt flow into the casting. When fronts of an oxidized surface meet and merge, oxide films are formed. The Smoothed particle hydrodynamics (SPH) method has an inherent advantage when tracking free surfaces and following complex flows, and thereby for studies of oxide and oxide film formation and transport. The SPH method is a grid-free, Lagrangian particle method where the continuum equations of fluid dynamics are replaced by particle equations [5]. The particles are the computational framework on which the fluid equations are solved and therefore, SPH automatically follow complex flows.

This study is a preliminary attempt to use the SPH method to study filling of a gravity die. Particles on the free surface are identified at all times of the filling process and the amount of oxides formed at the air exposed surface is estimated. A simple oxide growth model is employed for oxide formation. The subsequent transport of the oxides is analyzed. Furthermore, oxide films formed are identified and tracked as they moved with the melt.



2. Model description

Smoothed particle hydrodynamics (SPH) is a grid-free, Lagrangian method where the fluid is represented by a set of particles. Each particle carries fundamental physical properties, *e.g.* mass, position, velocity, density and other related properties. The value of any function f at a particle is approximated by summing over the properties of its neighbouring particles. The SPH interpolation of the function f of a particle i at position $\mathbf{r}_i$ is given by:

$$f(\mathbf{r}_i) \approx \sum_j \frac{m_j}{\rho_j} f_j W(\mathbf{r}_i - \mathbf{r}_j, h) \quad (1)$$

where index j corresponds to any neighbouring particle of particle i , m_j and ρ_j are the mass and the density for particle j , f_j is the value of f for particle j , the function W is an interpolation smoothing kernel, and h is a smoothing length that defines the radius of influence around the particle i . We use the Gaussian kernel function:

$$W_{ij} = \frac{C}{h^d} e^{-q^2} \quad (2)$$

where d is the dimension (2 or 3), $q = |\mathbf{r}_i - \mathbf{r}_j|/h$ and $C = 1/\pi$ for a 2D simulation and $C = \frac{1}{\sqrt{\pi^3}}$ for a 3D simulation. The radius of influence of this function is $3h$. It means that the particle i will not be affected by any neighboring particles farther than $3h$. The gradient of the function f is given by differentiating the interpolation equation (1) to give:

$$\nabla f(\mathbf{r}_i) \sim \sum_j \frac{m_j}{\rho_j} f_j \nabla_i W_{ij} \quad (3)$$

where

$$\nabla_i W_{ij} = \nabla W(\mathbf{r}_{ij}, h) = \frac{1}{h^2} \frac{\mathbf{r}_{ij}}{|\mathbf{r}_{ij}|} F(|\mathbf{r}_{ij}|, h) \quad (4)$$

and F is the derivative of the kernel function: $F(q) = -2C e^{-q^2}$.

2.1. SPH flow solver

The SPH fluid method is largely described in the literature [6, 7]. The governing equations of fluids in SPH method are based on the Navier-Stokes equations in the Lagrangian form. By using the SPH interpolation, the continuity equation describing the evolution of the fluid density over time can be written as:

$$\frac{d\rho_i}{dt} = \rho_i \sum_j \frac{m_j}{\rho_j} (\mathbf{v}_i - \mathbf{v}_j) \cdot \nabla W_{ij} + \chi_{ij} \quad (5)$$

where m and ρ_j are the mass and the density for particle j is the density for particle j , t is time and $\mathbf{v}$ is velocity. χ_{ij} is a density diffusive term introduced in Refs. [8, 9] which helps eliminate numerical noise.

The momentum equation describes the acceleration of the fluid and can be written as:

$$\rho \frac{d\mathbf{v}}{dt} = - \sum_j m_j \left(\frac{p_i}{\rho_i^2} + \frac{p_j}{\rho_j^2} - \frac{\xi}{\rho_i \rho_j} \frac{4\mu_i \mu_j}{\mu_i + \mu_j} \frac{\mathbf{v}_{ij} \cdot \mathbf{r}_{ij}}{r_{ij}^2 + \eta^2} + \pi_{ij} \right) \nabla W_{ij} + \mathbf{F}_i \quad (6)$$

where p is pressure, $\mathbf{F}$ is external force, μ_i is the dynamic viscosity of particle i and $\mathbf{v}_{ij} = \mathbf{v}_i - \mathbf{v}_j$. $\eta = 0.1h$ is used to prevent numerical divergence when two particles are approaching each other. ξ is the viscous scaling factor [10].

An equation of state is required to calculate the pressure in Eq.6. The equation of state used here is quasi-compressible form which is calculated by using the density information from Eq.5. The equation of state is given by:

$$p_i = \beta \left[\left(\frac{\rho_i}{\rho_0} \right)^\gamma - 1 \right] \quad (7)$$

where $\beta = c^2 \rho_0 / \gamma$ is the magnitude of the pressure, ρ_0 is the reference density, $\gamma = 7$ for liquid metal, and c is the speed of sound. The value of speed of sound should be large enough to ensure that the density fluctuation is less than 1% or close to the incompressible flow. The solid boundaries are represented by ghost particles as proposed in [8].

2.2. Oxide and oxide film formation

Prediction of oxide content is dependent on the ability to predict the amount of liquid metal exposed to air (*i.e.* metal located at the free surface) and the duration of that exposure. In SPH, each particle represents the same specific volume of fluid throughout the simulation and it can carry with it information on composition and the history of that particle. The oxide formation is calculated using the following key elements:

- Liquid metal particles oxidize for any period of time they are on the free surface. They do not oxidize when they are not currently on the free surface. This requires identification of which particles are on the surface at any time and an estimate of their exposed surface area.
- The rate of oxidation is given by a simple ordinary differential rate equation in this Lagrangian framework.
- Oxide already formed is transported by its host SPH particle to wherever it moves in the casting process.

The subsequent distribution of oxide produced by the fluid flow is therefore automatically provided by the method. The oxide content of any particle is given by a rate equation where k_l is the rate constant [11]:

$$\frac{dO_x}{dt} = k_l \quad (8)$$

The free surface is detected using the algorithm proposed in the work of Marrone et al. [12]. An algorithm is proposed to detect the oxide film during the simulation. When the normals of an oxidised surface are pointing against each other, oxide films is considered as entrained with the flow (as shown in Figure 1). Using the surface normal and the particle velocity, each surface can be detected and the algorithm can decide if a particle belongs to an oxide film.

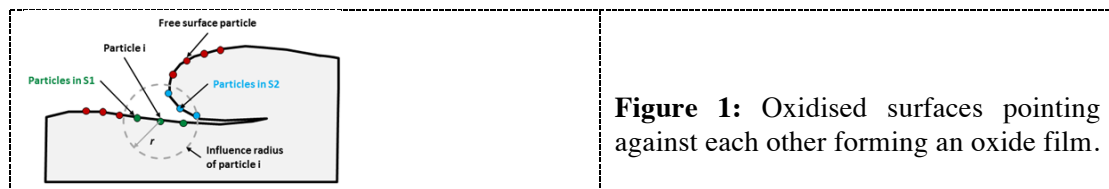


Figure 1: Oxidised surfaces pointing against each other forming an oxide film.

3. Case study

A 2D-model was set up to study filling of a gravity die (Fig. 2). The mould has a built-in pouring cup and ingate. The complete assembly is 150 mm high and 445 mm long. The die cavity has a length of 250 mm and has five steps with length of 50 mm and thickness of 30, 20, 15, 10 and 5 mm

respectively. The cavity is slightly inclined to up-hill flow and equipped with a feeder tube. The mould is filled by manually pouring metal into the cup.

The model includes the pouring cup, the ingate, the feeder and the die cavity (the mould is not included). The ghost particle technique was used to describe the solid boundary of the mould and a free slip boundary condition was used. The length of the pouring inlet was set to 16 mm and the center placed 5mm above the pouring cup. Two different pouring velocities were employed: 0,1 m/s and 0,4 m/s. Aluminium was modelled as a perfect liquid (Euler liquid) with a density of 2500 g/cm³. The particle size was set to 1mm giving 12500 particles in the filled die.

The constant k in the oxidation rate was set to 1, which means that the oxide content is equivalent to the air contact time. Oxide films formed when an oxidized surface folded and merged were identified and tracked as they moved along with the melt flow. The mould filling, the formation and transport of oxides and oxide films was analyzed for the two different inlet velocities.



Figure 2. The gravity die and the 2D-model of the gravity die.

4. Results

4.1. High pouring velocity

The total filling time for the case where the pouring velocity is set to 0,4 m/s is 2 seconds. The left panel of Figure 3 shows the flow field at different times during filling. The metal first hits the bottom of the pouring cup, partly flows down the ingate and partly fills up the pouring cup behind the metal jet. The metal flows along the mould bottom towards the steps, but circulates back towards the ingate until the bottom is completely filled up. The metal then enters the step part of the mould that gradually and smoothly fills up. When the steps are completely filled, excess metal is pushed upwards through the feeder. The flow velocity is highest through the ingate and is decreased when the metal hits the bottom of the mould.

Oxides will be formed at the free surface as the metal is exposed to air. The oxide content at different times during filling is shown in the left panel of Figure 4. An increased oxide level is found in the bottom of the mould before entering the steps. These oxides that are formed in the ingate and mould bottom, do not enter the steps, but are pushed up the feeder by the strong upward flow after the steps are filled. However, the free surface of the metal that enters the steps is also oxidized. The oxidized metal ends up in the upper part of the four thickest steps. The metal in step 5 (the thinnest step) has the highest oxidation level due to the long air exposure time of the metal that ends up in this step.

Oxide films are formed where two fronts (free surfaces) of the aluminum melt meet and merge. Oxide films are formed in the pouring cup, in the ingate and in the bottom of the mould where the flow velocities are high and creating melt splashing and circulating flow patterns. The oxide film content is shown in the right panel of Figure 3 at different times during filling. Most of the oxide films formed do not enter the steps, but are effectively transported toward the ingate with the circulating flow and finally pushed up the feeder after the steps are filled. As the steps fill up smoothly, oxide films are not formed within the steps. Some of the oxide films formed in the mold bottom are transported with the melt to the steps, and mostly end up in the upper part of the first and second step.

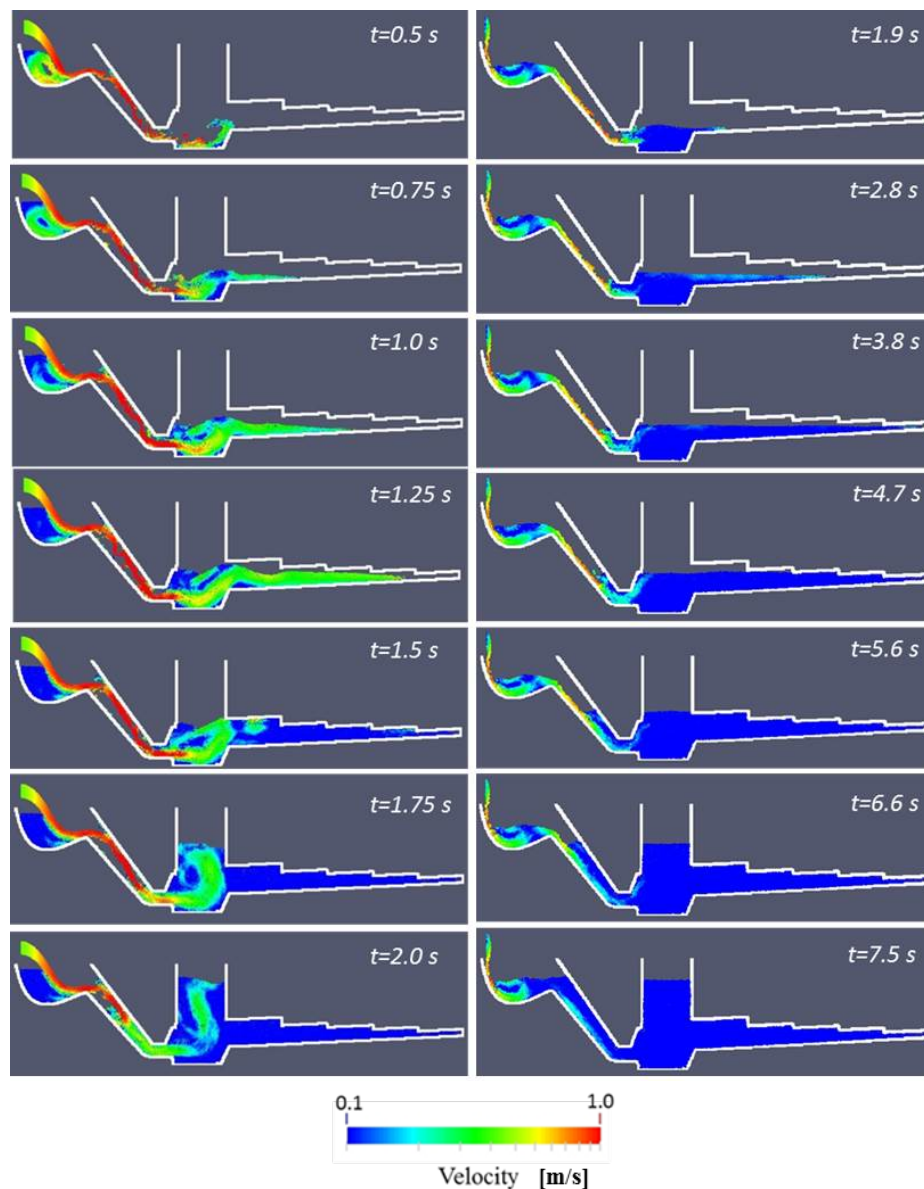


Figure 3. The velocity field (m/s) during filling when the velocity at the inlet is 0,4 m/s and 0,1 m/s in the left and right panel, respectively.

4.2. Low pouring velocity

The total filling time for the case where the pouring velocity is set to 0,1 m/s is 7.5 seconds. The right panel of Figure 3 shows the flow field at different times during filling. The metal first flows along the wall of the pouring cup, it circulates counter clockwise in the cup and when the cup is filled the melt flows down the ingate without filling it up. The melt reaches the bottom of the mould that fills before the melt can enter the step part. The melt velocities are highest in the ingate and at the entrance to the mould. The velocities in the mould bottom are low, but fronts are merging as the melt circulates counter clockwise towards the ingate. When the steps start to fill, the melt also flows from the mould bottom and up the ingate that fills up simultaneously. As the ingate fill up, the melt that enters the mould is pushed upwards along the mould walls to the melt surface. The metal smoothly fills up the step part of the mould. When the steps are completely filled, excess metal fills up the feeder.

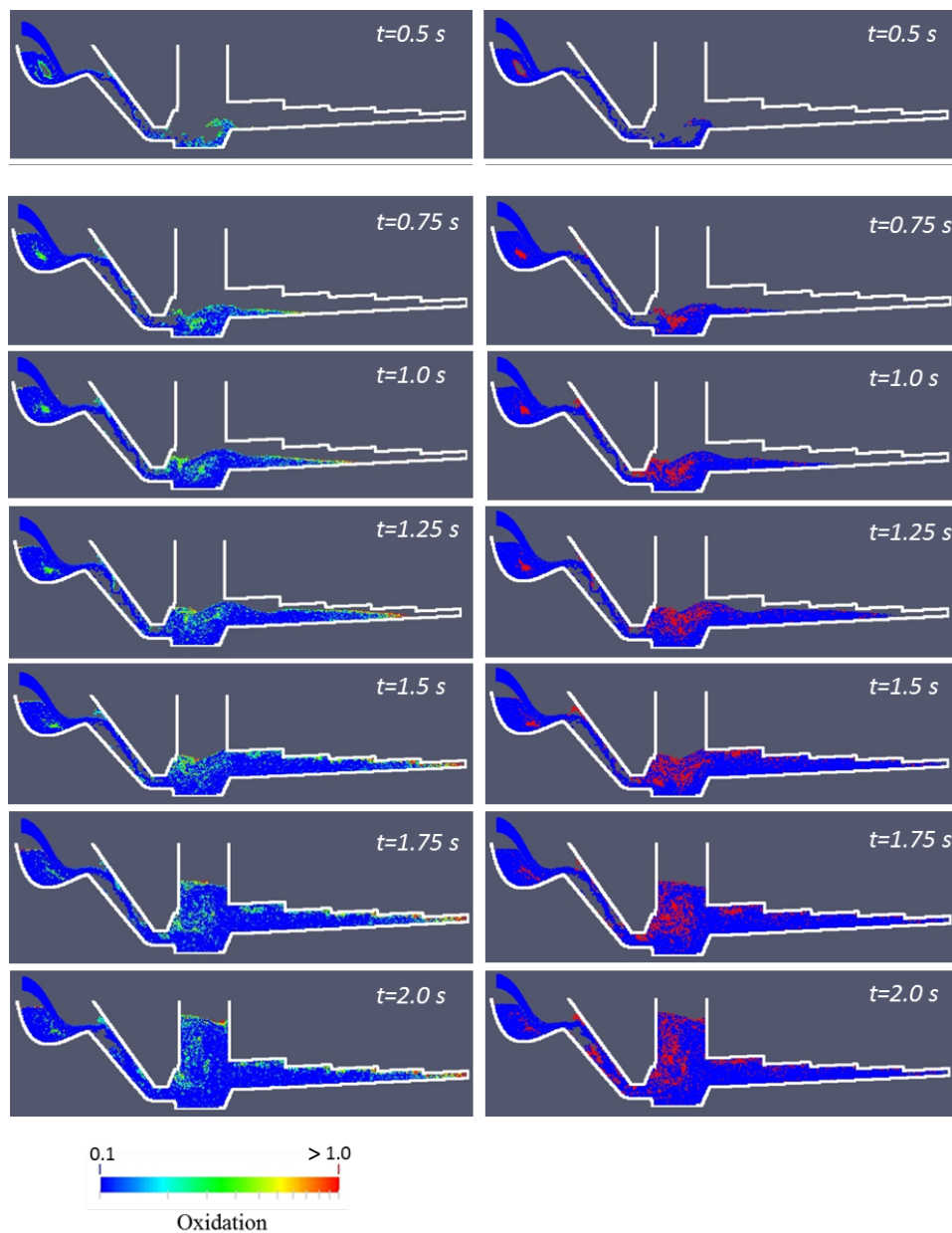


Figure 4. The left panel shows oxidation level during filling when the velocity at the inlet is 0,4 m/s. The right panel shows the corresponding oxide films (marked in red).

The oxide content at different times during filling is shown in the left panel of Figure 5. Elevated oxide content is found in the melt in the bottom of the mould before the melt enters the steps. These oxides are transported towards the melt surface and then flow with the melt into the steps. As the melt enters the steps, the surface is further exposed to air and the oxidation level increases. As the filling time is longer than for the case with high pouring velocity, the exposure time is longer. The metal that fills up the thinnest steps (4 and 5) is highly oxidized. High oxide content is also found in the thicker steps. The oxide film content is shown in the right panel of Figure 4 at different times during filling. Oxide films are formed in the pouring cup and the bottom of the mould due to the circulating flow patterns in these parts. The oxide films are transported to the melt surface in the mould bottom before entering the step part of the mould. As the steps fill up smoothly, oxide films are not formed within

the steps. Very few oxide films ends up in the thinnest step, but the four remaining steps have a high oxide film content. The oxide films ending up in the feeder are formed after the step part of the mould is filled.

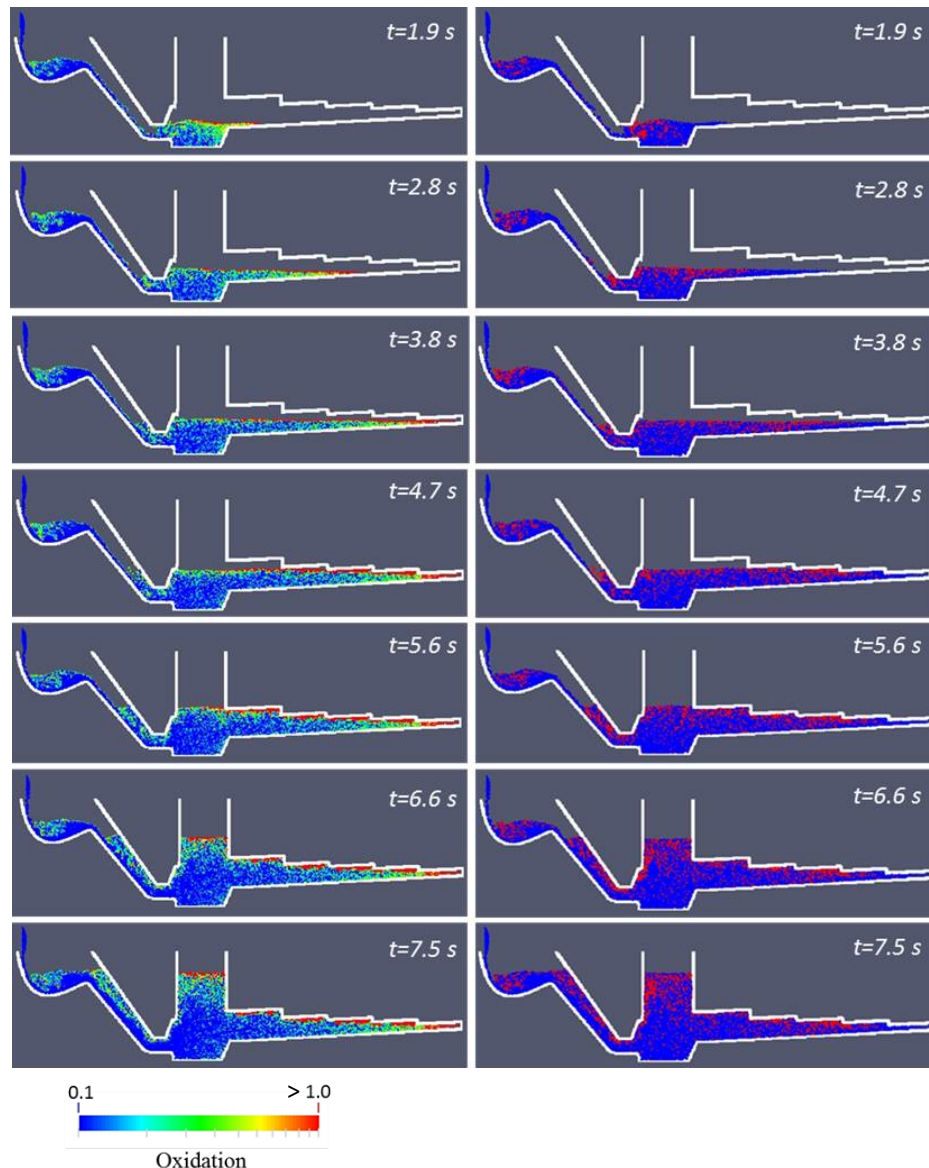


Figure 5. The left panel shows the oxidation level during filling when the velocity at the inlet is 0,1 m/s. The right panel shows the corresponding oxide films (marked in red).

5. Discussion and summary

The oxidization level is higher in the case with low pouring velocity. The free surface has a longer air exposure time when pouring the melt slowly and the filling time is longer. Furthermore, it has been demonstrated that for the higher pouring velocity, the high melt velocity obtained in the mould bottom creates a melt flow pattern that transport oxides effectively towards the feeder. The oxidation level is highest in the thinnest step for both cases as the melt transported to this step has the longest air exposure time. For the case with high pouring velocity the four other steps have a low oxidation level, for the low pouring velocity the oxidation level increases with decreasing thickness and increasing distance from the ingate due to the increasing air exposure time for the free surface of the melt

entering the step. The steps in the case with low pouring velocity fill up smoothly and the flow velocity is low. A lower formation rate of oxide films is therefore expected compared to the case with higher pouring velocity. However, the oxide film content is higher in all steps for the low pouring velocity case. This is due to the formation of oxide films in the pouring cup and mould bottom and the subsequent transport towards the step part of the mould. In the case with high pouring velocity, the melt flow patterns leads to transport of oxide films towards the ingate in a circular pattern away from the steps and finally to the feeder. The SPH method is tracking free surface flows with fragmentation and breakup more accurately than is possible with traditional grid based methods [13] and the Lagrangian framework of the method allows tracking of history-dependent properties such as accumulated oxide mass [14]. The preliminary study demonstrates the usefulness and the potential of using the SPH method for studies of melt filling, oxide and oxide film formation and transport. The method can be used to increase the understanding of the effect of different filling procedures on the cast quality.

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