FRONT TRACKING METHOD FOR SIMULATION OF SOLIDIFICATION PROCESSES WITH PURE ALUMINUM

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Abstract

Solidification process plays an important role in the production of metallic materials. Conditions of this process considerably determine mechanical properties of semi-finished products. Nowadays, metallurgists frequently utilize computational solidification models that enable the numerical investigation of solidification. Most of these tools are based on interface capturing methods, which are straightforward and quite easy for implementation. However, a main drawback of these methods is their accuracy in the determination of the moving interface separating the phases. The paper presents the front tracking method, which enables to overcome the mentioned issues. Pure aluminum, which solidifies at a constant temperature, is considered in the study. The front tracking method, the enthalpy method, the effective heat capacity method and the temperature recovery method are used for simulations. Results gained with the use of computational approaches are compared to an exact solution of a 1D Stefan problem. Conclusions of the study indicate that the front tracking method is a very accurate tool and has a potential for investigation of the microstructure.

Keywords: Front tracking**,** aluminum, Stefan problem, solidification, numerical modelling

1. INTRODUCTION

Nowadays, the replacement of steel by aluminum or aluminum alloys is an often discussed topic. Mainly in automotive industry the use of aluminum can decrease the weight of automobiles. This approach has positive impacts to the car control and helps to increase the fuel efficiency and to reduce CO_2 emissions. For instance, in September 2015 Ford Motor Company announced that Ford and its major suppliers work together on a new material known as Micromill, which represents a new aluminum alloy. Future demands for aluminum by automakers are expected to grow annually by 30 % till 2020 [1]. However, the mechanical properties and durability of aluminum parts have to be equivalent as in case of made of steel. The microstructure of a material formed during the solidification process considerably influences the overall quality. Knowledge, how the crystals grow from the melt and which parameters influence the crystal growth, is potentially very useful. Pure aluminum, which solidifies at a constant temperature, may be formed by two major distinct zones, columnar and equiaxed dendrites [2]. The zone of columnar dendrites, which advance into the liquid, emerges in the vicinity of ingot walls with high temperature gradients. On the other hand, equiaxed dendrites originate within the locally undercooled melt and they grow outward from their origin in all directions [3]. In practice, the most demanded materials are usually those with the equiaxed structure as it has uniform mechanical properties. However, in some special cases, the columnar structure is also required.

During the solidification of aluminum a large amount of latent heat is released. The latent heat must be considered in a computer model in order to obtain accurate and reliable results. In general there are two basic concepts of numerical solutions to phase change problems [4]. The first approach includes interface capturing methods where an additional or modified quantity is introduced to the heat transfer equation in order to model the release and/or accumulation of the latent heat [5]. The interface capturing methods have widely been used in engineering and science as they are simple and they can be easily implemented in computer programs. The typical representatives of the interface capturing methods are the well-known enthalpy method, the effective

heat capacity method, the temperature recovery method and combinations of these. The interface capturing methods are well suited for non-isothermal phase transformation but they do not allow for explicit tracking of the interface between the phases. In contrary, the position of the interface has to be determined afterward from the temperature distribution. In general, the interface capturing methods suffer from low accuracy in the determination of the temperature distribution, and especially in the interface location. The second approach to modelling of the heat transfer problems with phase changes includes the interface tracking, so-called front tracking methods. In these methods the accurate position of the interface between the phases (the solid and liquid phases in case of aluminum solidification) is determined explicitly at each time step. The release or accumulation of latent heat is incorporated by means of the Stefan condition. The front tracking methods allow for a significantly higher accuracy, mainly in the determination of the interface location. However, the front tracking methods are computationally more complicated and demanding, especially in 3D.

In the paper the mentioned interface capturing and interface tracking approaches are investigated. The 1D case with the heat transfer is considered. Other phenomena, e.g. fluid flow, are not taken into account. Results for the solidification process of pure aluminum are evaluated and compared with the 1D exact solution to the Stefan two-phase problem. The results show that front tracking method is a promising tool for a precise investigation of the moving interface and heat transfer in solidifying metals.

2. EXACT SOLUTION TO THE STEFAN TWO-PHASE PROBLEM

A Stefan problem is a heat transfer problem with phase changes. Since the problem includes the front separating the phases, the problem is often referred to as the moving interface problem [6]. The heat transfer with the phase change can be mathematically described in one spatial dimension by the governing equation

$$\rho c_p \frac{\partial T}{\partial \tau} = \frac{\partial}{\partial x}\left(k_{eff} \frac{\partial T}{\partial x} \right) + \rho L \frac{\partial f_s}{\partial \tau}, \tag{1}$$

where c_p (J/kg·K) is specific heat, ρ (kg/m^3) is density, k_{eff} (W/m·K) is effective thermal conductivity, T (K) is temperature, L (J/kg) is latent heat, f_S (1) is the solid fraction, τ (s) is time and x (m) is the spatial coordinate.

Only a limited number of phase change problems can be solved analytically. These mainly include 1D cases of an infinite or semi-infinite regions with constant thermophysical properties and simple boundary conditions. An isothermal (at a constant temperature T_m) phase change is assumed in the exact solution to the Stefan problems. The exact solution to the Stefan two-phase problem is of the following form [6]

$$\frac{T_S(x,\tau) - T_0}{T_m - T_0} = \frac{\operatorname{erf}\left\{ x / 2(\alpha_S \tau)^{1/2} \right\}}{\operatorname{erf}(\lambda)} \qquad \frac{T_L(x,\tau) - T_i}{T_m - T_i} = \frac{\operatorname{erfc}\left\{ x / 2(\alpha_L \tau)^{1/2} \right\}}{\operatorname{erfc}\left(\lambda (\alpha_S / \alpha_L)^{1/2} \right)}, \tag{2}$$

where T_S is the temperature in the solid phase, T_L is the temperature in the liquid phase. The temperatures T_0, T_m, T_i are the temperature at the boundary, the phase change temperature and the initial temperature, respectively, and α (m^2/s) is the thermal diffusivity. The location of the interface is determined from the Stefan condition balancing the phases

$$k_S \left. \frac{\partial T_S}{\partial x} \right|_{x=s(\tau)} - k_L \left. \frac{\partial T_L}{\partial x} \right|_{x=s(\tau)} = \rho L \frac{ds(\tau)}{dt} = \rho L v_n \tag{3}$$

as $s(\tau) = 2\lambda\sqrt{\alpha_L \tau}$ where the parameter λ is the solution of the transcendental equation, see e.g. [6].

3. NUMERICAL METHODS

Various numerical methods discussed in the introduction were employed to build numerical models. The finite difference method with the use of the explicit formula for the time derivate was used for the numerical discretization of Eq. (1).

3.1. Enthalpy method

In the enthalpy method, the latent heat of the phase change is included in a new thermodynamic quantity - the enthalpy [7]. The enthalpy is used as the primary variable and the temperature is calculated from a defined enthalpy-temperature relationship. The Eq. (1) with the use of the enthalpy reads

$$\rho \frac{\partial h}{\partial \tau} = \frac{\partial}{\partial x}\left(k_{eff} \frac{\partial T}{\partial x} \right) \qquad h = \int_0^T \left(c_p - L \frac{\partial f_S}{\partial \psi} \right) \mathrm{d}\psi \,, \tag{4}$$

where h (J/kg) is the enthalpy. The enthalpy method has some advantages in comparison to other methods. It ensures the energy conservation at all times since the enthalpy is solely increasing with the increasing temperature. Further, there is no discontinuity at either the liquidus or solidus temperatures. However, the enthalpy method is computationally more demanding and also more difficult to implement, mainly in case of the implicit numerical scheme.

3.2. Effective heat capacity method

The effective heat capacity is a very often used method in solidification/melting modelling. In this method, the latent heat is included in the artificially increased specific heat in the phase change temperature range [8]. The latent heat can be calculated by the integration of the effective heat capacity over the temperature interval. The effective heat capacity is related to the enthalpy as its derivative with respect to the temperature as shown in Eq. (5). The Eq. (1) with the effective heat capacity method can be formulated as

$$c_{eff} \rho \frac{\partial T}{\partial \tau} = \frac{\partial}{\partial x}\left(k_{eff} \frac{\partial T}{\partial x} \right) \qquad c_{eff} = \frac{\partial h}{\partial T} = c_p - L \frac{\partial f_S}{\partial T} \,, \tag{5}$$

where c_{eff} (J/kg·K) is the effective heat capacity. Since the heat capacity can be regarded as the temperature-dependent quantity, the implementation of Eq. (5) into a computer program is straightforward. The weak point of the effective heat capacity method is the difficulty related to the fulfilment of the energy conservation. In particular, in case the computed temperature jumps over the phase change temperature range within one time iteration, the latent heat is not taken into account. Other techniques are therefore required to overcome such issue.

3.3. Temperature recovery method

In this method, the temperature at which the phase change occurs is considered as in the absence of latent heat. After each time step the temperature crossing the phase change is set back to the phase change temperature and the equivalent amount of latent heat is added to the enthalpy budget for a particular node. Once the local enthalpy budget z_i equals to the latent heat corresponding to the volume associated with the node, the temperature is allowed to decrease [9]. The Eq. (1) can be reformulated with the use of the temperature recovery method to the form

$$c_p \rho \frac{\partial T}{\partial \tau} = \frac{\partial}{\partial x}\left(k_{eff} \frac{\partial T}{\partial x} \right) \qquad z_i = L\left(\frac{1}{c_L} + \frac{1}{c_S} \right) \Big/ 2. \tag{6}$$

If the temperature T^* drops below the melting temperature T_m, the local enthalpy budget is updated according to $z_i = z_i - (T^* - T_m)$ and the temperature T^* is replaced by the phase change temperature T_m until $z_i > 0$. The main advantage of this approach, in comparison to the effective heat capacity method, is that the phase change is not complete until all the latent heat of phase change is released or absorbed. This implies that the conservation of energy is ensured. This method is also computationally economic and easy to implement. However, the method is very sensitive to the size of the time step and errors in the solution peaks in the vicinity of the phase change temperature than in the single phase regions.

3.4. Front tracking method

In comparison to interface capturing methods, the primary goal of the front tracking method is a precise determination of the interface between the phases [10]. The solution for the temperature distribution is determined in the second step. This is the opposite order than in case of interface capturing methods. The interface, the so-called front, and its movement are monitored with a special care. The front tracking method employs the fixed grid domain and the front moves within it. The method is therefore referred to as the mixed Eulerian-Lagrangian approach. The front is represented by mass-less markers (see **Figure 1**), which are situated on grid lines of the domain. As time goes by and the temperature distribution evolves, the markers move within the grid in the direction normal to the front [11]. The normal velocity v_n of the markers is calculated explicitly with the use of the Stefan condition given in Eq. (3), which expresses the energy balance at the interface. When the markers are advected within the time iteration, the front needs to be reconstructed and new marker lying on the grid lines have to be determined as shown in **Figure 1**. The front separates the domain into two regions in which the temperature distribution is solved separately and independently of each other.

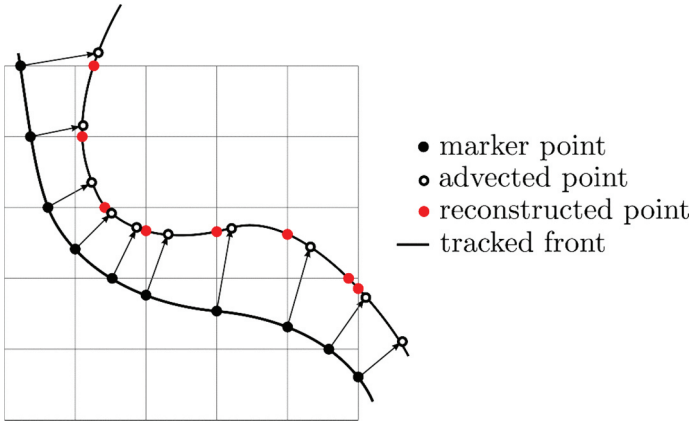

Figure 1 Scheme of the front tracking method

4. RESULTS AND DISCUSSION

A 1D study case was chosen to investigate the accuracy of the methods presented in Section 3. The exact solution presented in Section 2 was used for the evaluation. The study case consisted of aluminum, which solidified from the temperature 750 °C. The phase change temperature was set to 660 °C and the Dirichlet condition was employed at the boundary prescribing the surface temperature of 620 °C. Zero heat flux was assumed at the other boundary. The length of the domain was 3 m and the simulations were carried out for the solidification process lasting 1 hour of the wall clock time. The accuracy of the numerical methods was compared with the exact solution to the investigated Stefan problem by means of the mean temperature error and the mean front position error defined as follows

$$\text{mean temperature error} = \frac{1}{n}\sum_{i=1}^{n}\left|T_i - T_i^*\right| \qquad \text{mean front position error} = \frac{1}{m}\sum_{j=1}^{m}\left|s_j - s_j^*\right|, \tag{7}$$

where T is the calculated (simulated) temperature, T^* is the exact temperature, s is the calculated (simulated) front position, s^* is the exact front position, n = 400 represents the number of spatial nodes and $m = 10^5$ is the number of time steps (iterations). The results are presented in **Table 1** and shown in **Figure 2** and **Figure 3**.

As can be seen in **Figure 2**, all the methods used for simulations provide a relatively precise prediction of the temperature distribution within the investigated aluminum domain. A detail of the temperature distribution around the phase change temperature shown in **Figure 2** reveals that there are some minor discrepancies in case of all the interface capturing methods. On the other hand, the front tracking method allowed for more precise results. In particular, the mean temperature errors for the methods are presented in **Table 1**. In case of interface capturing methods, the mean temperature error varies from 0.0318 °C (the temperature recovery method) to 0.1006 °C (the effective heat capacity method). Though these temperature errors are relatively small, the mean temperature error for the front tracking method is even significantly smaller, only 0.0015 °C.

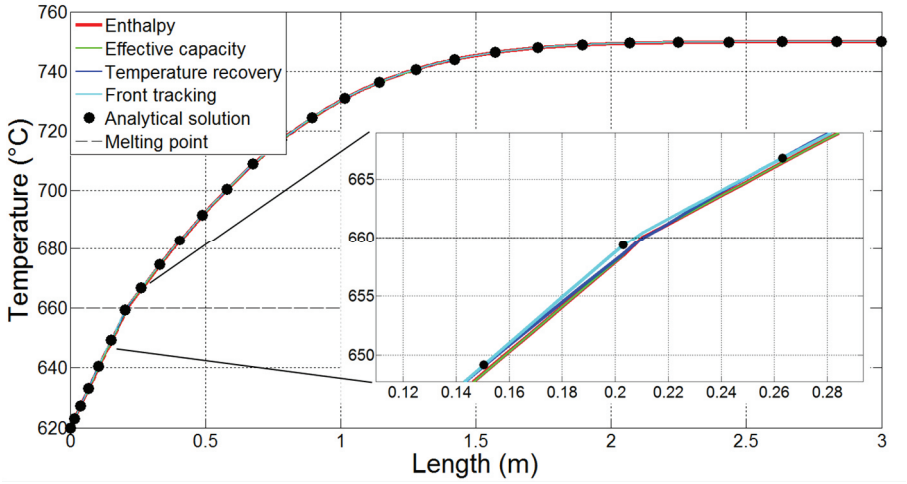

Figure 2 Temperature distributions in the aluminum domain at the final time of simulation (1 hr)

More interesting results are presented in **Figure 3** where the location of the solidification front is shown. As expected from the experience and confirmed with the exact solution, the front location is a smooth function increasing with time as the front propagates. However, as can be seen in **Figure 3** all the interface capturing methods behave in a different manner. In particular, the front location is incorrectly determined as a step function instead of a monotonically increasing function, see the detail in **Figure 3**. Such behaviour is due to the nature of the interface capturing methods. The reason for this is the spatial discretization of the domain into nodes, each pertaining to a certain volume of the material. In simulation, some nodes and their volumes have the temperature close to the phase change temperature, which causes inaccuracy in the determination of the front location. Further, discrepancies also originate from the nature of the interface capturing methods as the front location is determined as a consequence of the temperature distribution.

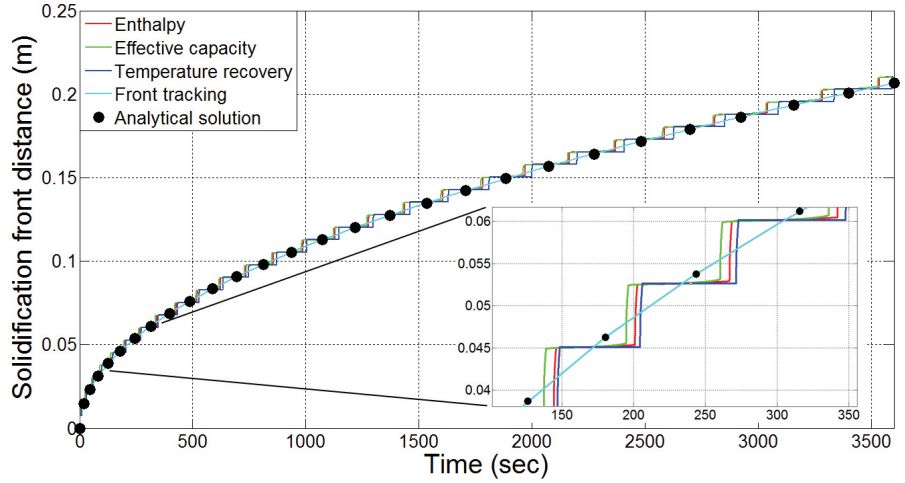

Figure 3 Location of the solidification front as a function of time

On the other hand, the front tracking method allows for a very precise determination of the front location, see **Figure 3**. This is a feature of the front tracking method and the high accuracy is attained since the front is tracked explicitly by means of the Stefan condition. The temperature distribution is determined as a consequence of the front location. This is a reverse order than in case of the interface capturing methods. The very high accuracy can also be evaluated by means of the mean front location error presented in **Table 1**. The mean error in the front location is almost 20 mm in case of all the interface capturing methods. However, the front tracking method has the mean error of the front location of only 0.037 mm. This implies that the solid-liquid interface can be tracked very precisely. The front tracking method is therefore a promising tool for the

detailed analysis of the solidification and the method will be further employed for the prediction of the micro-structure. Especially in 3D it is expected that the front tracking method can provide much more precise results than interface capturing methods.

Table 1 Mean errors - discrepancies between the exact and simulated results

Measure of accuracy	Numerical method			
	Enthalpy	Eff. heat capacity	Temp. recovery	Front tracking
Mean temperature error	0.0897 °C	0.1006 °C	0.0318 °C	0.0015 °C
Mean front location error	19.144 mm	19.754 mm	18.621 mm	0.037 mm

5. CONCLUSION

The front tracking method was developed for the solution of heat transfer problems with phase changes. The method was used with three well-known interface capturing methods for the simulation of the aluminum solidification. The exact solution of the 1D Stefan problem was employed for the validation. The simulated results revealed that all the methods allow for a relatively precise determination of the temperature distribution but interface capturing methods fail in the determination of the interface location, which separates the phases. On the other hand, the front tracking method allows for the very precise determination of the front location and the method is therefore promising for development of simulation tool of the micro-structure.

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