A direct method of solidification for the enhancement of mushy zone network models

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Abstract

Network models allow to study fluid flow around numerous grains during solidification. It appears that the predicted behavior of a network model depends heavily on the rate of solidification estimated for each individual channel. Therefore, a suitable 1D solidification model is investigated with direct methods. The model includes heat, solute and mass conservation as well as the Wilson–Frenkel formula. An accurate but CPU-time consuming method is presented.
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Keywords: Network modeling; Simulation; Solidification

1. Introduction

In order to get a better understanding of the fluid flow through the mush at high solid fractions a network model was recently developed [1]. Its main idea is to represent the liquid by a set of geometrical simplified channels. The individual channel widths are adapted in accordance to the solidification or melting process.

For a good prediction of permeability within a network model it is therefore essential to have a fast but yet accurate estimate of the amount of solidification. In a most simple situation the network will contain channels formed by parallel planes. In this case it is for symmetry reason enough to consider the 1D solidification of a slab which is solid on one side and liquid on the other side.

For the application within a network model the following three criteria have to be met. Firstly, the model must be fast. The reason for this is that network models require a huge amount (usually thousands) of channels.

Secondly, as long as a 1D solidification is enough for the inclusion within a network model, all things related to surface tension and the Gibbs–Thompson relation can be neglected. However, in certain situations, inclusion of shrinkage upon solidification was found crucial for the outcome of the network simulations. Therefore, a model including density changes of the liquid and solid should be preferred.

Thirdly, conservation of heat, solute and mass should be treated equally. Especially, whether changes of heat or solute induces solidification should not be determined in advance. Within network models it is likely that convection of solute from upstream channels influences solidification, on the other hand the production of latent heat of fusion determines in many cases the solid–liquid interface temperature.

In consequence of these criteria it was decided to use a direct method, i.e. a front tracking method based on finite difference or collocation which determines new solute and temperature profiles while at the same time the amount of heat, mass and solute at the interface is conserved.

In literature only few models meet with above three criteria. The model proposed in the rest of this articles is as far as the authors know not described elsewhere. There exist however two similar models. The one described by Galenko and Zhuravlev [2] is based on the same set of conservation equations but uses an averaging technique to find a solution near the liquid–solid interface. The other is described by P. Zhao et al. [3]. It differs from the one described here by using a

generalized Gibbs–Thompson relation and standard weighted residuals.

2. Model description

For the rest of this article a 1D slab with domain [0,1] is considered. Initially, the left half part of the slab with domain [0,0.5] is solid, and the other part is liquid (see Fig. 1). Upon solidification the solid part will grow and the solid–liquid interface will move to the right.

2.1. Constitutional equations

The common basis of all solidification models are the conservation equations. They can be expressed in several forms. Here the from as derived in [4] is used. Within the solid and liquid heat and solute conservation can be expressed as

$$\frac{\partial T_\alpha}{\partial t} - a_\alpha \Delta T_\alpha = 0, \tag{1}$$

$$\frac{\partial C_\alpha}{\partial t} - D_\alpha \Delta C_\alpha = 0. \tag{2}$$

Here the temperature T_α is either the temperature in the liquid, i.e. for $\alpha = l$ or the temperature in the solid (for $\alpha = s$). The same holds for the solute concentration C_α. D_α is the diffusion constant of the liquid or solid and a_α is the thermal diffusivity in the liquid or solid.

Even though conduction of heat is on the scale of dendrites comparatively fast, no thermal equilibrium was assumed. It was observed that accurate transport of the latent heat produced at the solid–liquid interface is crucial for the determination of the interface velocity.

At the solid–liquid interface I; mass, solute and heat are conserved as well. Using mass conservation two additional interface equations can be derived out of the conservation of solute and
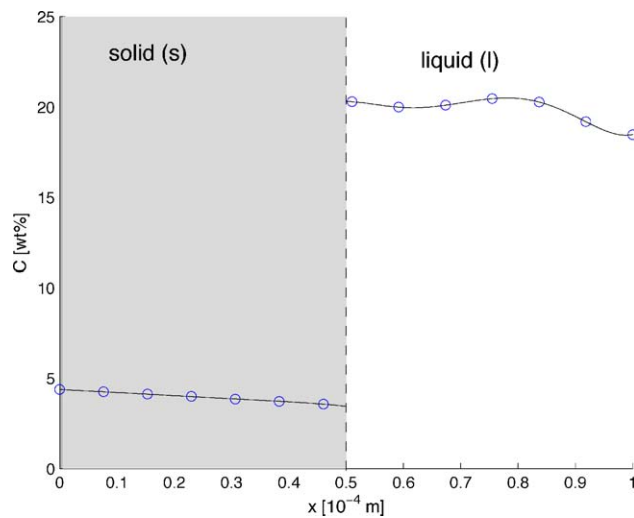

Fig. 1. Initial solute concentration profile in the liquid and solid. This is the profile next figures shows predicted interface values for. The collocation points are indicated.

heat:

$$v \left(k - \frac{\rho_s}{\rho_l} \right) = D_l \left. \frac{\partial C_l}{\partial x} \right|_{x=I^-} - D_s \left. \frac{\partial C_s}{\partial x} \right|_{x=I^+}, \tag{3}$$

$$v(\rho_l - \rho_s) c_{p_l} T_l \big|_{x=I^+} - v\rho_s L = \kappa_l \left. \frac{\partial T_l}{\partial x} \right|_{x=I^-} - \kappa_s \left. \frac{\partial T_s}{\partial x} \right|_{x=I^+}. \tag{4}$$

In these last equations ρ_s and ρ_l are the solid and liquid densities, κ_s and κ_l the conductivity in the solid and liquid which are not be mistaken for the partition coefficient k (see Eq. (7)). Furthermore, c_{p_l} is the specific heat within the liquid while, L is the latent heat of fusion. It is indicated whether the derivative of the solute or liquid profile has to be taken.

The velocity v of the interface will be determined by the Wilson–Frenkel formula, which for a small undercooling δT at the interface can be approximated [5] by

$$v = \beta \delta T. \tag{5}$$

This equation couples conservation of solute and heat at the interface with the help of the kinetic coefficient β.

Finally at the interface the temperature on both sides of the interface remains the same while the solute concentration has a discontinuity, i.e. at the solid–liquid interface:

$$T_s|_{x=I^-} = T_l|_{x=I^+}, \tag{6}$$

and

$$C_s|_{x=I^-} = kC_l|_{x=I^+}. \tag{7}$$

2.2. Numerical solution

In order to find a numerical solution for the concentration and temperature field which satisfies above equations, a collocation method is used. That is, the solutions are represented by the weighted sum of a complete set Bernstein-polynomials [6] which form a low order polynomial basis.

For the liquid and for the solid part two completely separate basis and sets of weight coefficients are used. The domain of both polynomial basis was taken to include the whole liquid and solid part. This rather unconventional approach seems to have no serious disadvantages as long as the interface is near the middle and the collocation points are chosen only in the liquid or solid part, respectively. It avoids however unnecessary transformation of the basis polynomials.

An additional Landau-transformation is avoided. Instead, the liquid and solid fields are re-interpolated at the new collocation points which are lineary distributed. The collocation method together with a Backward–Euler scheme allows to write Eqs. (1) and (2) in discrete form.

To fulfill the requirements of the remaining interface conditions two alternatives are possible. Either Eqs. (3) and (4) are reformulated in terms of residuals R_1, R_2:

$$R_1 = \left| v \left(k - \frac{\rho_s}{\rho_l} \right) - D_l \left. \frac{\partial C_l}{\partial x} \right|_{x=I^+} + D_s \left. \frac{\partial C_s}{\partial x} \right|_{x=I^-} \right|, \tag{8}$$

$$R_2 = \left| v(\rho_1 - \rho_s)\, c_{p_1} T_1 \big|_{x=I^+} - v\rho_s L - \kappa_1 \frac{\partial T_1}{\partial x} \bigg|_{x=I^+} \right.$$
$$\left. + \kappa_s \frac{\partial T_s}{\partial x} \bigg|_{x=I^-} \right|, \tag{9}$$

which are then minimized, or both equations together with Eqs. (7) and (6) are discretized as well (in accordance to the already used collocation method) and an overdetermined system of equations has to be solved.

3. Observations and discussions

3.1. Residual method

With the residuals minimization procedure the trial functions are found by first choosing the liquid and solid solute concentrations and temperatures at the interface such that Eqs. (6) and (7) are fulfilled. Then the liquid and solid profiles can be determined using Eqs. (1) and (2). If the choice of interface concentrations and temperature was optimal, the residuals (8) and (9) are zero.

For all simulations the physical constants of Al–Cu alloys where used (with the exception of β) as can be found in [1]. It was observed that with these constants the residuals depend nearly linear on the choice of interface concentrations and temperature. This means that when the velocity of the interface is already known new solution profiles will be found after the generation of the sixth trial.

A new interface velocity can be determined by the requirement of self consistency, i.e. the interface concentrations and temperature are varied till both residuals (8) and (9) are zero at the same time.
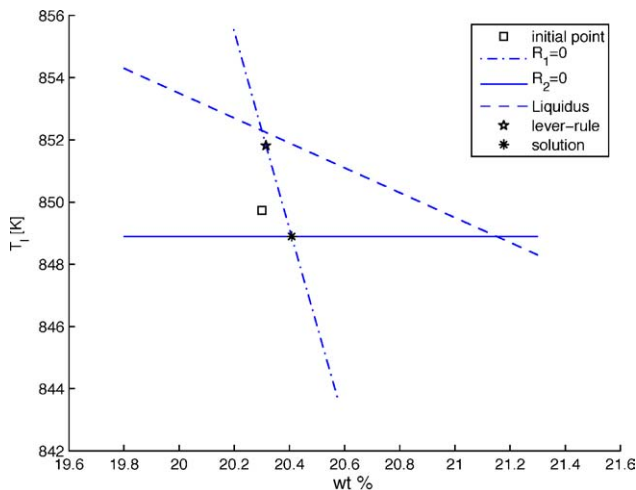

Fig. 2. Phase-diagram of Al–Cu alloys showing possible concentrations and temperatures after solid–liquid interface movement. While the conduction of heat and its interface condition $R_2 = 0$ allow in this region only for one interface temperature, the prediction of the interface concentration ($R_1 = 0$) depends on the actual undercooling. A self-consistent solution is found when both fields predict the same interface temperature and concentration. As indicated, this is not the same point as predicted with application of local lever rule.
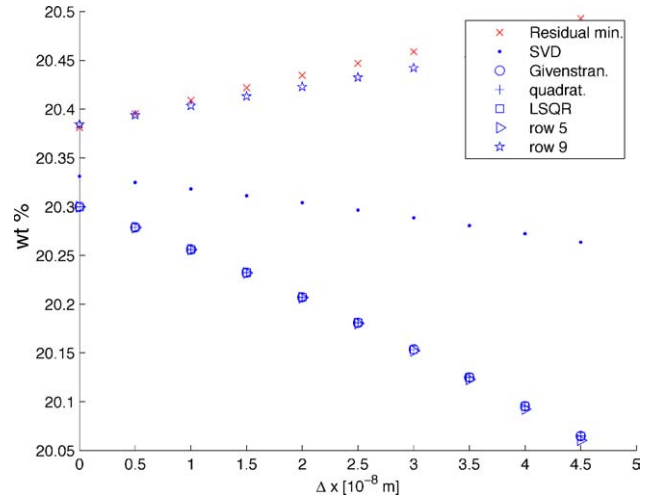

Fig. 3. Predicted interface concentrations in dependence to the distance of interface movement. The results of various standard methods capable of solving the overdetermined equation system are shown. Following methods were used: singular value decomposition (SVD), Givens transformation (Givenstran.), Quadrature method (quatrat.), and LSQR method (LSQR). Furthermore, the result of the substitution of the fifth (row 5) and ninth (row 9) row with the interface equation (3) and the result obtained from the residual minimization process are shown as well.

As can be seen in Fig. 2 this very CPU-time consuming process cannot really be enhanced by local application of the lever rule around the interface. It was checked that this deviation was not due the lack of conservation of solute. The total loss or gain of the solute content was determined numerically to be less than 0.1%, which is expected due to diffusion and conduction.

3.2. Other methods

If Eqs. (1)–(4), (7) and (6) are linearized all together an overdetermined system of linear equations is obtained. It has been tried to solve this system by standard methods [6], i.e. using singular value decomposition, quadrature method, LSQR method, and Givens transformation. The solutions showed however not to coincide with the result of the minimizing of residuals (see Fig. 3).

Best results were found when two of the discretized equations (1) and (2), respectively, were replaced by the interface equations. This does not always work well because the system can become singular depending on the amount of interface movement.

4. Conclusions

A model for 1D simulation of solidification which includes the Wilson–Frenkel formula has been presented. It has been shown that the model can be solved by using a direct method. Finally it has been indicated that some other (more obvious) direct methods might fail.

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