



Temperature-based energy solver coupled with tabulated thermodynamic properties – Application to the prediction of macrosegregation in multicomponent alloys



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ARTICLE INFO

Article history:

Received 17 September 2014
Received in revised form 4 December 2014
Accepted 6 December 2014
Available online 12 January 2015

Keywords:

Finite element method
Energy conservation
Thermodynamics
Solidification
Macrosegregation

ABSTRACT

We present a new algorithm for solving energy balance in phase change problems, particularly in solidification with macrosegregation. The algorithm is based on a nonlinear temperature evaluation using the average enthalpy which is provided by (i) tabulated phase transformation paths and (ii) tabulated phase properties. The compatibility of this method with tabulations using a thermodynamic database, allows simulating solidification at equilibrium with multiple phase transformations for binary and multicomponent alloys. The method has been validated and applied to three-dimensional cases with macrosegregation: a binary Sn–3 wt.% Pb alloy and a ternary Fe–2 wt.% C–30 wt.% Cr alloy. For the latter case, predictions include composition maps for C and Cr due to thermosolutal instability leading to freckle formation and the subsequent distributions of liquid, BCC, FCC, M_7C_3 and Cementite phases. Compared with a previously published enthalpy method, the temperature-based energy solver shows similar accuracy and faster computational time.

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1. Introduction

Macrosegregation, a well distinguished defect in alloy solidification, has been a main research topic in the metallurgy community for the last few decades [1]. It develops within several physical scales: at a microscopic scale, solute partitioning between the liquid and solid phases creates composition gradients at the interface between the phases, known as microsegregation [2]. Macroscopically, fluid flow in the liquid phase as well as other mechanical factors, such as deformation of the mush [3,4], solidification shrinkage [5] and transport of grains [6,7] may redistribute unevenly the rejected chemical species. These transport phenomena gradually enrich or deplete the melt located outside an established mushy zone, leading to regions with significant composition differences, hence altering the properties in the finished product. To model macrosegregation, a minimum of four conservation principles are used: conservation of mass, momentum, chemical species and energy. The phase change literature contains a wealth of numerical methods to solve energy conservation in solidifying alloys. A comprehensive overview of these methods is given by Swaminathan and Voller [8]. The corresponding equation associates the total average enthalpy to the temperature via intrinsic

alloy properties, such as the heat capacity of the phases and the latent heat associated with the phase transformations. However, in the course of solidification with macrosegregation, these properties may change because the average composition may vary significantly: the transformation paths are then modified, as well as the phases' composition and heat capacity. Similarly, the latent heat of phase transformations is not a constant that could be distributed as a function of the phase fractions assuming only temperature-dependent phases' properties, as often found in the literature [9]. It is thus impossible to establish a priori the dependence of the enthalpy with respect to temperature when macrosegregation takes place, even in the case of full thermodynamic equilibrium between phases.

The current work discusses a suitable numerical scheme based on an enthalpy method, already used in the literature to alleviate this macrosegregation-related problem [8,10]. Secondly, we introduce a modified formulation, using the effective heat capacity method that increases the original scheme's efficiency. The current method is thus an enthalpy method that makes use of a temperature-based solver. Moreover, it uses tabulated thermodynamic quantities (solidification paths, phases' enthalpy and composition) in a range of average compositions and temperatures as found in the literature [11–13], with the aim of evaluating the total average enthalpy as well as the effective heat capacity. The novelty of the modified method resides in the use of thermodynamic tabulations

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without losing the advantages of the previous method, thus yielding faster computation times while maintaining a good accuracy. Finally, test cases are presented.

2. Thermodynamic considerations

2.1. Volume averaging

A volume averaging technique was suggested to deal with the presence of multiple phases [14]. It locally considers a Representative Volume Element (RVE) that contains several phases at a mesoscopic scale. We represent, for each unknown ψ , an intrinsic volume average, $\langle \psi \rangle^\phi$ (also denoted $\langle \psi^\phi \rangle^\phi$ in the literature), corresponding to a phase ϕ . The volume average $\langle \psi \rangle$ for this unknown in the RVE, hence averaged over all the present phases writes:

$$\langle \psi \rangle = \sum_{\phi} g^{\phi} \langle \psi \rangle^{\phi} \quad (1)$$

where g^{ϕ} denotes the volume fraction of phase ϕ in the RVE. It should be emphasized that the averaging technique applies to virtually all thermodynamic variables (enthalpy, density, etc.). Among these variables, the temperature is considered to be uniform in the RVE. Applying the volume averaging technique to the energy conservation principle along with interfacial balances between the phases, results in the following averaged equation [15]:

$$\frac{\partial(\rho h)}{\partial t} + \nabla \cdot (\rho h \mathbf{v}) = \nabla \cdot (\kappa \nabla T) + \dot{Q}_v \quad (2)$$

where ρ stands for the density, h the mass enthalpy, \mathbf{v} the velocity field, κ the thermal conductivity, T the temperature and \dot{Q}_v a possible volume heat source. While the latter source is zero in the rest of this contribution, we keep it to maintain a general formulation of the energy conservation. Eq. (2) is the standard averaged form of the energy conservation equation used in non-stationary phase change problems. Once the variational form has been discretized in space and time, two possible resolution schemes emerge: the first is an explicit forward Euler scheme which gives rise to a linear equation where the temperature denoted by T^t is known at time t . This requires very small time steps in the current context, which limits the solver's usability at the scale of industrial applications. The second scheme is the backward Euler or full implicit discretization where terms are function of $T^{t+\Delta t}$. It leads to a nonlinear equation with 2 interdependent unknowns, $\langle \rho h \rangle^{t+\Delta t}$ and $T^{t+\Delta t}$. It is clear that the nature of the temperature–enthalpy relationship plays a central role when formulating the resolution strategy of this nonlinear equation. Generally, it is admitted that, depending on the resolution strategy, it is necessary to express enthalpy as a function of temperature or vice versa, together with associated partial derivatives, $d\langle \rho h \rangle / dT$ or $dT / d\langle \rho h \rangle$.

2.2. The temperature–enthalpy relationship

In solidification problems, additional variables are involved in Eqs. (1) and (2), like the transformation path that defines the history of the phase fractions, as well as the average chemical composition $\langle w_i \rangle$, i being the index of the chemical species (only the solutes are considered). The temperature–enthalpy relation averaged over the phases in a given RVE writes:

$$\langle \rho h \rangle = \sum_{\phi} g_{(T, \langle w_i \rangle, \dots)}^{\phi} \langle \rho \rangle_{(T, \langle w_i \rangle, \dots)}^{\phi} \langle h \rangle_{(T, \langle w_i \rangle, \dots)}^{\phi} \quad (3)$$

Note that the volume average enthalpy is approximated by the product $\langle \rho h \rangle^{\phi} = \langle \rho \rangle^{\phi} \langle h \rangle^{\phi}$ in the current work. As stated in the introduction, it becomes clear from Eq. (3) that phase properties, i.e. average phase density, $\langle \rho \rangle_{(T, \langle w_i \rangle, \dots)}^{\phi}$, and enthalpy, $\langle h \rangle_{(T, \langle w_i \rangle, \dots)}^{\phi}$, are

temperature and composition dependent. This equation is the key to convert the average volume enthalpy to temperature (through a procedure named H2T) or vice versa (T2H). The values of the different phase fractions g^{ϕ} (solidification path) and phase enthalpies $\langle \rho h \rangle^{\phi}$ are thus needed to close the relation.

2.3. Tabulation of properties

The complexity of performing a thermodynamic conversion is directly linked to the simplicity of determining the alloy properties, namely the phase fractions and phase enthalpies. In the case of binary alloys and with several assumptions with respect to the system (e.g., linear monovariant temperature–composition relationships, constant heat capacity of phases and constant latent heat of transformations, equilibrium approximations between phases) analytical calculations are often used to determine the properties. Nevertheless, analytical relations are more complex or even impossible to derive in the case of multicomponent alloys ($i > 1$). To overcome this problem, one can resort to thermodynamic databases and phase equilibrium calculations to tabulate the transformation paths and the phase enthalpies for a given range of temperatures and average compositions. It is a handy solution for two main reasons: first, the conversion is merely a binary search in a table; secondly, it is a simple solution for coupling with macrosegregation. In this way, phase fractions g^{ϕ} are tabulated as functions of temperature and average composition, while for each phase ϕ the mass enthalpy, $\langle h \rangle^{\phi}$, and the density, $\langle \rho \rangle^{\phi}$, are tabulated as functions of temperature and phase intrinsic average compositions $\langle w_i \rangle^{\phi}$, as well as other possible parameters. Fig. 1 summarizes the steps in order to perform a temperature-to-enthalpy (T2H) conversion using the predefined tabulation approach. In step 1, the transformation path is acquired for each average composition and temperature to determine the list of phases, their volume fractions g^{ϕ} and their intrinsic compositions $\langle w_i \rangle^{\phi}$. In step 2, the phase enthalpy $\langle h \rangle^{\phi}$ and density $\langle \rho \rangle^{\phi}$ are determined by searching for the temperature and the already known phase composition $\langle w_i \rangle^{\phi}$. In step 3, the average volume enthalpy is computed from the volume fraction, density and mass enthalpy of phases using Eq. (3).

The methodology to build the tabulations is straightforward. It is based on two main scans. On the one hand, intervals for the variation of the average composition $\langle w_i \rangle$ are chosen from the known alloy composition. These variations have to cover the extreme values adopted during the simulation, which are not known a priori. An interval is also selected for the variation of temperature. The latter is easier to determine as it usually starts from the initial melt temperature and goes down to the room temperature in a standard casting simulation. For these intervals, a systematic scan is made with chosen steps in each composition and T , during which a thermodynamic equilibrium is computed. The outputs are the number of phases encountered, together with their fraction and intrinsic composition. The minimum and maximum intrinsic composition for each phase could then be determined. On the other hand, for each phase, a scan of the intrinsic composition and temperature is made to compute the intrinsic properties. The same temperature interval and step as defined earlier are used. This strategy based on full thermodynamic equilibrium means that it is limited to the so-called lever rule approximation.

Regarding the enthalpy-to-temperature conversion (H2T), a backward iterative T2H search is performed. For a known composition $\langle w_i \rangle$, denoting k the iteration index to convert the enthalpy $\langle \rho h \rangle_{\text{input}}$, we start with an initial guess for temperature $T^{(k=0)}$ then convert it to an enthalpy $\langle \rho h \rangle^{(k)}$ with the T2H conversion. Using an appropriate nonlinear algorithm (Brent is the most versatile in our case), we aim at minimizing the following residual:

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