Modeling and Simulation of Macrosegregation Induced by Thermomechanical Deformation in Steels

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1 Introduction

Metallurgical processes have known a great evolution during the last 60 years. The advancement is attributed to research disciplines, like physical metallurgy, which investigated a great deal of solidification-related phenomena. Nowadays, metallurgists and physicists seek to understand deeper the connection between the different scales involved. From the nucleation theory to the mechanical behavior of metals, an chain of intricate phenomena occur in a such a way to create defects in the final product. This has been seen in casting processes like continuous casting and ingot casting. Suface and volume porosity, hot tearing and composition heterogeneities are known defects to the casting community. As far as the current project is concerned, the last defect, widely known as macrosegregation, is the subject of our interest.

Defects

> Worth checking notes from the Ecole Thématique CNRS oléron (Check Mail Draft)

- Hot tearing

- Porosity

- Freckles

- Macrosegregation

Industrial Worries

Production

- Talk about total steel production, variations over the last few decades

- Quality constraints for many applications that require steel like construction, nuclear engines ?

- Difficulties to meet these constraints and what are the present solutions

Research and Simulation

- Need for software handling multicomponent alloys

1   • Need for software handling finite diffusion in the solid

2   • Need for realistic alloy properties (not only constants)

3   • Need for handling moulds along with volume change (creating thermal resistances)

> Worth discussing Isabelle Poitraut and David Cardianaux - and Claudine Allentin (respo comm
> Arcelor Dunkerque, search for mail)

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CCEMLCC contribution

6   • some words about this ESA project

7   • in what ways does this project tries to alleviate the aforementionned problems ?

8   • academic and industrial partners and how does each of them contribute actually

9   • mention *Thercast* as the final developped code destination ?

Chapter 1

Modelling Review

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In this chapter the following points are discussed

- what does a typical solidifications problem consist of ? heat - fluid - solid - chemical species

- what are the modeling scales of these physics ? direct (micro: phase field / macro: CA) and indirect (micro Nancy models / macro: current FE model)

> Maybe worth showing the 2x2 table that CAG showed at the ICASP conference ?

- Overview of these models ??

- Presence of AIR requires a new problem definition : Lagrangian or Eulerian framework

1.1   Standard FE model

A section presenting the main FE equations along with their weak formulations that will be solved in the metal being a single domain. I call it "standard" because it doesnt contain anything about levelsets, compressibility, ...

- Energy (chapter 1)

- Species mass (voller prakash)

> should I mention the tabulation approach that I couldnt finalize because of the equality between w and wl in liquid phase ?

- Fluid mechanics (vms: darcy model with boussinesq)

> talking about Eulerian approach Air Metal will be presented in the next chapters, it should be the biblio section of another chapter

1.2   Biblio test

[**?**] are going to appear in the paper

Chapter 2

Energy Resolution: Tsolver

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When we speak about macrosegregation in solidification, we have to remember that the problem is one that involves phase change.

2.1 State of the art

- Use of enthalpy resolution in the majority of works

- motivation and advantages of TvsH without talking about resolution time

- use article's introduction to fill this section (or improvise new things)

2.2 Thermodynamic considerations

> this section should be revised for missing symbols, equations and figures from the corresponding article

2.2.1 Volume averaging

A volume averaging technique was suggested to deal with the presence of multiple phases [1]. It locally considers a Representative Volume Element (RVE) that contains a single or several phases (these are not necessarily in thermodynamic equilibrium) at a mesoscopic scale. We represent, for each unknown ψ, an intrinsic volume average, HERE (also denoted HERE in the literature), corresponding to a phase HERE. The volume average HERE for this unknown in the RVE, hence averaged over all the present phases writes: HERE Eq. 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 …). Among these variables, the temperature is also 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 [2]: HERE Eq. 2 where ρ stands for the density, h the mass enthalpy, v the velocity field, κ the thermal conductivity, T the temperature and Q_V a possible volume heat source. 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 is known at time t, T^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, $\frac{d\langle \rho h \rangle}{dT}$ or $\frac{dT}{d\langle \rho h \rangle}$.

2.2.2 The temperature-enthalpy relationship

In solidification problems, additional variables are involved in Eq. 1 and Eq. 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: HERE Eq. 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, , HERE and enthalpy, HERE, 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.

2.2.3 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 HERE, as well as other possible parameters. Figure 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.

FIGURE 1 (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.

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 HERE with the T2H conversion. Using an appropriate nonlinear algorithm (Brent is the most versatile in our case), we aim at minimizing the following residual: HERE. Once the algorithm has converged, the temperature $T^{(}(k))$ is the result of the H2T conversion. It is inferred that the first conversion (T2H) is a direct one whereas the latter (H2T) is indirect and requires a series of iterative steps; each step being a single T2H resolution. In other words, a H2T conversion is a backward search for a temperature, hence it's slower. This conversion's speed lag is exacerbated when tabulations increase in size (e.g. large number of temperature and composition steps) and complexity (e.g., multicomponent industrial alloys used in casting), since the search gets more complicated with the increasing number of input columns (one column for each alloying element).

2.3 Formulation

from HvsT article

Bibliography

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[2] Michel Rappaz, Michel Bellet, and Michel Deville. *Numerical Modeling in Materials Science and Engineering*. Springer Series in Computational Mathematics. Springer Berlin Heidelberg, 2003.

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