Modeling and Simulation of Macrosegregation Induced by Thermomechanical Deformation in Steels

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Contents

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

- Need for software handling finite diffusion in the solid

- Need for realistic alloy properties (not only constants)

- 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)

CCEMLCC contribution

- some words about this ESA project

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

- academic and industrial partners and how does each of them contribute actually

- mention *Thercast* as the final developped code destination ?

Chapter 1

Modelling Review

Contents

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

[5] are going to appear in the paper

Chapter 2

Energy Resolution: Tsolver

Contents

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 [10]. 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, $\langle\psi\rangle^\phi$ (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:

$$\langle\psi\rangle = \sum_\phi g^\phi \langle\psi\rangle^\phi \tag{2.1}$$

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 [11]:

$$\frac{\partial\langle\rho h\rangle}{\partial t} + \vec{\nabla}\cdot\langle\rho h\vec{v}\rangle = \vec{\nabla}\cdot\left(\langle\kappa\rangle\vec{\nabla}T\right) + \langle\dot{Q}_V\rangle \tag{2.2}$$

where ρ stands for the density, h the mass enthalpy, $\vec{v}$ the velocity field, κ the thermal conductivity, T the temperature and $\dot{Q}_V$ a possible volume heat source. Equation 2.2 is the standard averaged form of the energy conservation equation used in non-stationary phase change problems.

> I could elaborate more in this paragraph by showing the possible equations for the explicit formulation and maybe a figure to show the AlSi7 computation that i did with a v small time step

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 Equation 2.1 and Equation 2.2, 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:

$$\langle\rho h\rangle = \sum_\phi g^\phi_{(T,\langle w_i\rangle...)}\rho^\phi_{(T,\langle w_i\rangle^\phi...)} h^\phi_{(T,\langle w_i\rangle^\phi...)} \tag{2.3}$$

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 Equation 2.3 that phase properties, i.e. average phase density, , ρ^ϕ and enthalpy, h^ϕ, 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, h^ϕ, and the density, ρ^ϕ, 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 h^ϕ and density ρ^ϕ 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 Equation 2.3.

Figure 3 goes here

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.

below paragraph should be re written and maybe stress LESS on the speed effect

I should change the superscript k which may be confused with partition coefficient

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 $\langle \rho h \rangle^{(k=0)}$ with the T2H conversion. Using an appropriate nonlinear algorithm (Brent is the most versatile in our case), we aim at minimizing the following residual: $\text{Residu}_{\langle \rho h \rangle} = \left| \langle \rho h \rangle_{\text{input}} - \langle \rho h \rangle^{(k)} \right|$. 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

Coming soon

2.4   Validation

2.4.1   Pure diffusion

The two solvers are first tested in a purely diffusive case for a one-dimensional solidification configuration. Predictions with a 1D front tracking model [7] is used as a benchmark. It provides solutions for the temperature and solid fraction during directional solidification of a 10 cm long Al – 7 wt.% Si ingot. The melt, with initial uniform temperature, is cooled with a heat exchange coefficient (assuming a Fourier boundary condition) from one side, the other side being adiabatic. All values for alloy properties, initial and boundary conditions and numerical parameters are listed in Table 2.1. For this simple test case, we use linear temperature dependence of the intrinsic phase enthalpies, that is $\langle \rho h \rangle^s = \langle \rho C_p \rangle T$ and $\langle \rho h \rangle^l = \langle \rho C_p \rangle T + \rho L$, where $\langle \rho C_p \rangle$ is the heat capacity per unit volume and ρL is the latent heat per unit volume. Values for $\langle \rho C_p \rangle$ and ρL, as well as for the thermal conductivities, $\kappa = \langle \kappa^l \rangle = \langle \kappa^s \rangle$, are taken constant. Moreover, a Gulliver Scheil approximation is used to compute a single temperature – fraction of solid relationship in the absence of macrosegregation. This is done assuming a linear binary phase diagram and thus requires using the properties listed in Table 2.1, i.e. the segregation coefficient, k, the liquidus slope, m_L, the liquidus temperature, T_L, and the eutectic temperature, T_E. **Figure REF** shows the comparison with the Hsolver and Tsolver. The results are found superimposed to the front tacking solution, thus giving validation of the implementation as well as the iterative schemes presented above to solve the energy conservation.

2.4.2   Convection-diffusion with macrosegregation

Conservation equations in **Table 2** are for mass, momentum and chemical species. As for energy, they are presented after the volume averaging technique has been applied [10] [6]. Moreover, an assumption of a static and non deformable solid phase is made. Consequently, the mechanical model is reduced to the conservation of momentum in the liquid phase. This assumption also yields some other consequences on the mass balance and the liquid momentum conservation. In the latter, a Darcy term is added to take into account the dissipative interfacial stress in the porous-like mushy zone. Its main parameter is the permeability of the mushy zone, K. It is considered isotropic, hence reducing to a scalar which is given by the Carman-Kozeny relation, based on the secondary dendrite arm spacing $\lambda_2 : K = \frac{g^{l3} \lambda_2^2}{180 \left(1 - g^l\right)^2}$. The liquid density being taken constant, its spatial variations as a function of temperature and average composition are still needed to compute thermosolutal convection forces. For that purpose, the Boussinesq approximation $\langle \rho \rangle^l = \rho_{\text{ref}} \left(1 - \beta_T \left(T - T_{\text{ref}}\right) - \beta_{\langle w \rangle^l} \left(\langle w \rangle^l - w_{\text{ref}}^l\right)\right)$ is used, considering the thermal β_T and solutal $\beta_{\langle w \rangle^l})$ expansion coefficients and a reference density, ρ_{ref}, defined at a reference temperature T_{ref} and reference composition w_{ref}^l. Values

Parameter	Symbol	Value	Unit
Nominal composition	$\langle w \rangle_0$	7	•
Liquidus temperature	T_L	618	•
Eutectic temperature	T_E	577	•
Segregation coefficient	k	0.13	•
Liquidus slope	m_L	−6.5	•
Heat capacity (liquid and solid)	ρC_p	2.6×10^6	•
Enthalpy of fusion	ρL	9.5×10^8	•
Thermal conductivity (liquid and solid)	κ	70	•
Heat transfer coefficient	h_{ext}	500	•
External temperature	T_{ext}	100	•
Initial temperature	T_0	800	•
Ingot length		0.1	•
FE mesh size		10^{-3}	•
Time step	Δt	0.1	•
Convergence criterion (residual)	ε_R	10^{-6}	•
Convergence criterion (temperature)	ε_T	10^{-2}	•

Table 2.1: Parameters for the pure diffusion test case with alloy Al – 7 wt.% Si presented in **FIGURE REF**

for the references are taken at the liquidus temperature and the nominal composition of the alloy, $\langle w \rangle_0$ [5]. More details about the FE formulation can be found in [12, 4]. It should be noted that the macroscopic solute diffusion coefficient in the solid phase is neglected in **REF Eq. 15c**.

> in this table I use directly the simplified equations, but this was done only for the article, now I have to go from the full conservation equations and state the hypothesis and methods that i used to reach this simplified form

$$\nabla \cdot \left(g^l \, \vec{v}^l \right) = 0 \tag{2.4a}$$

$$\frac{\partial}{\partial t} \left(g^l \rho_{\text{ref}} \vec{v}^l \right) + \vec{\nabla} \cdot \left(g^l \rho_{\text{ref}} \vec{v}^l \times \vec{v}^l \right) - \vec{\nabla} \cdot \langle S \rangle^l - g^l \nabla p^l + \mu^l g^{l^2} K^{-1} \vec{v}^l - g^l \rho^l \vec{g} = 0 \tag{2.4b}$$

$$\frac{\partial}{\partial t} \left(\langle w_i \rangle \right) + \left(g^l \vec{v}^l \right) \cdot \vec{\nabla} \langle w_i \rangle^l + \nabla \cdot \left(g^l D^l \vec{\nabla} \langle w_i \rangle^l \right) = 0 \tag{2.4c}$$

Table 2.2: Averaged conservation equations for the conservation of mass (a), momentum (b) and solute mass (c)

> Figure SMACS: Computed unidirectional heat diffusion during solidification of an Al – 7 wt.% Si alloy using (orange) the enthalpy method and (black) the temperature method, comparison being made for (left) cooling curves and (right) time history of the liquid fraction. Each curve corresponds to a position along the sample, from 0 cm (cooling side) to 10 cm (insulated side), with 2 cm spacing between the positions.

The Tsolver's ability to be coupled with various physical phenomena like macrosegregation and fluid flow in porous medium is displayed in this test case. It consists of a solidification

benchmark where a 10 cm width × 6 cm height × 1 cm thick cavity containing a Sn – 3 wt.% Pb melt is cooled down from its two narrowest vertical sides using heat exchangers (LHE: left heat exchanger, RHE: right heat exchanger). The experiment, inspired by Hebditch and Hunt's [9] similar set up, has been revisited by Hachani et al. [8] who performed the solidification with better controlled conditions and using an increased number of samples for composition analysis. Recently, a successful attempt to simulate the experiment was carried out by Carozzani et al. relying on an enthalpy resolution [5]. All details regarding geometry, finite element discretization, material properties and boundary conditions can be found in the latter reference.

I could develop more here giving additional details

For this computation, solidification paths, phase compositions and phase enthalpies were determined by a thermodynamic module dedicated to equilibrium calculations for binary alloys. The 3D simulation results in **REF Figure 4** show a satisfactory agreement with the experimental temperature measurements recorded at mid heights of the cavity and uniformly distributed along its width [5]. In fact, simulation results with the Tsolver and the Hsolver were found to be almost superimposed, as in **REF Figure 4**. Regarding the computation, the Tsolver resolution proves to be faster than the Hsolver used in [5]: a process time of 7000s required a computation time of 90 hours 13 minutes compared to 114 hours 21 minutes spent by the enthalpy resolution with 32 cores on the same cluster. The gain factor is about 20%.

2.5 Application to multicomponent alloys

The efficiency of the temperature-based resolution resides in its performance when combined with thermodynamic tabulations. A multicomponent alloy consists of at least two solute elements, and therefore the tabulation size increases, hence the number of search operations also increases. To demonstrate the speed-up ability of the temperature-based approach while predicting all phase transformations during macrosegregation, we consider the solidification of a ternary alloy, Fe–2 wt.%C– 30 wt.%Cr. As illustrated in **Figure 5a**, the alloy domain has a cylinder shape close to 3-inch height × 1-inch diameter. Exact values are reported in **Table 3** with all material properties, initial and boundary conditions, as well as numerical parameters for the simulations. The melt steel is initially at 1395 °C. The temperature of the bottom surface is imposed with a constant decreasing rate of 0.1 K.s-1 starting with 1380 °C, i.e. 40 °C higher than the nominal liquidus temperature, as shown in **Figure 5b**. The other surfaces are kept adiabatic. The cylinder is held in a vertical position. In these conditions, and knowing that the carbon and chromium solutes have lightening effects on the liquid at nominal composition, the density inversion resulting from the composition gradient in the interdendritic liquid, may cause flow instability (segregation plumes) at the solidification front. While the selected alloy is a steel, this application is also representative of directional cooling in a single crystal casting, e.g. for nickel-base superalloys [3]. **Figure 5c** also provides the transformation path of the alloy at nominal composition, i.e. assuming no macrosegregation and full thermodynamic equilibrium as computed with ThermoCalc and the TCFE6 database [2, 1]. A total of 5 phases need to be handled, the characteristic temperature for their formation being reported in

Figure 5b.

> Figure 5: Configurations for directional casting of (a) a 1 inch diameter × 3 inches height cylin-
> drical domain for which (b) temperature-time conditions are imposed at its bottom surface.
> The alloy is Fe – 2 wt.% C– 30 wt.% Cr, its computed transformation path [20], [21] at nominal
> composition being displayed in (c)

2.5.1   Tabulations

Full thermodynamic equilibrium is considered in the present case. Due to macrosegregation,
the average composition is expected to continuously vary in time and space during casting.
Transformation paths are thus determined a priori for a set of average compositions around
the nominal value. Hence, carbon content is arbitrarily varied in the interval [1.8 wt.%, 2.2
wt.%] while chromium content variation is in the interval [27 wt%, 33 wt%]. The offset of ±10%
with respect to the nominal composition value allows tabulating relatively small composition
steps to ensure a good accuracy when compared to the corresponding ternary phase diagram.
The average composition step is 0.04 wt.% for carbon and 0.6 wt.% for chromium, thus
representing 2% intervals with respect to the nominal composition. The temperature varies in
the interval [100 °C,1600 °C] by 5 °C steps. For each triplet (carbon content in wt.% C, **HERE** ,
chromium content in wt.% Cr, **HERE**, temperature in K) corresponds a phase fraction g^{ϕ} and
a pair of intrinsic phase composition (**HERE**). For the 5 phases listed in **Figure 5c** (LIQ≡liquid,
BCC≡ferrite, FCC≡austenite, M7C3≡carbide, CEM≡cementite), the enthalpy h^{ϕ} and density
ρ^{ϕ}, are tabulated as functions of temperature and phase intrinsic composition. If this latter
input lies between two tabulated values, a linear interpolation is performed to determine
the output, i.e. phase enthalpy and density. With the advancement of solidification, the
liquid is enriched with solute by macrosegregation, which enables new solidification paths. It
means that the primary solidifying phase is not necessarily the same as when considering the
nominal composition. For this reason, the tabulation approach is interesting inasmuch as it
provides phase transformation paths and values of phase properties that are compatible with
the system's actual composition. **Figure 6** summarizes the tabulated thermodynamic data for
two sets of average composition for the considered ternary system. Note that in the present
test case, phase densities are taken constant ($\rho^{s} = \rho^{l} = 6725 \, \text{kg m}^{-3}$). Therefore they are not
tabulated. With this assumption, no shrinkage occurs upon phase change.

Parameter	Symbol	Value	Unit
Nominal composition	$\langle w_C \rangle_0$	2	wt.%
	$\langle w_{Cr} \rangle_0$	30	wt.%
Characteristic temperatures	T_{top}, T_{bottom}	**FIGURE**	°C
Phase fraction	g^ϕ	Tabulations	–
Phase enthalpy	$\langle h \rangle^\phi$	Tabulations	–
Phase composition	$\langle w_C \rangle^\phi$	Tabulations	wt.%
	$\langle w_{Cr} \rangle^\phi$	Tabulations	wt.%
Diffusion coefficients	$\langle D_C \rangle^l$	•	$m^2\,s^{-1}$
	$\langle D_{Cr} \rangle^l$	•	$m^2\,s^{-1}$
Dynamic viscosity	μ^l	2×10^{-3}	Pa s
Thermal expansion coefficient	β_T	•	K^{-1}
Solutal expansion coefficient	$\beta_{\langle w_C \rangle^l}$	•	wt.%$^{-1}$
	$\beta_{\langle w_{Cr} \rangle^l}$	•	wt.%$^{-1}$
Thermal conductivity in the solid	•	•	$W\,m^{-1}\,K^{-1}$
Thermal conductivity in the liquid	•	•	$W\,m^{-1}\,K^{-1}$
Dendrite arm spacing	•	•	m
Density	•	•	$kg\,m^{-3}$
Initial temperature	•	•	°C
Ingot diameter	•	•	m
Ingot length	•	•	m
FE mesh size		10^{-3}	m
Time step	Δt	0.1	s
Convergence criterion (residual)	ε_R	10^{-6}	–
Convergence criterion (temperature)	ε_T	10^{-2}	K

Table 2.3: Parameters for solidification of alloy Fe – 2 wt.% C – 30 wt.% Cr

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