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Modelling and simulation of ingot solidification with the open-source software *Code_Saturne*

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Abstract. In order to address the issue of macro-segregations in large industrial ingots, a solidification model has been recently developed in *Code_Saturne*, the general purpose open-source Computational Fluid Dynamics (CFD) software developed and released by EDF R&D. This model is a liquid-solid mixture model inspired from the pioneer work of Bennon and Incropera, including mass, momentum, energy and species conservation equations. In particular, the energy conservation equation is formulated with the temperature variable, the thermosolutal convection is accounted for through the Boussinesq approximation and the interdendritic flow in the mushy zone is governed by the Darcy's law. Furthermore, a rigid solid phase is assumed and classical microsegregation models are used featuring lever-rule or Gulliver-Scheil assumptions. At the discrete level, a first-order upwind scheme is implemented with a SIMPLEC approach to solve the velocity-pressure coupling. The other couplings involving temperature and concentration fields are efficiently solved performing sub-loops with a PISO-like approach. The overall scheme is mainly implicit with additional treatments to ensure the equilibrium between the hydrostatic pressure gradient and the buoyant forces, and to deal properly with solid zones. The segregation predictions offered by the model are validated against both academic test case and industrial ingot configurations. A convergence study is also led focusing on time step and mesh size sensitivities.

1. Introduction

Ingot casting is a manufacturing process widely used in several industries including automotive, naval, aeronautic, petroleum or nuclear industry. The ingot results from a phase change where a liquid phase, generally an alloy, becomes solid. This phase change generally takes place over a range of temperatures, thus solid and liquid can coexist in equilibrium at various temperatures. The co-existence of both phases is macroscopically regarded as a mushy zone, where the solid phase forms a porous matrix through which the residual liquid flows. In the mushy zone, the liquid phase is enriched compared to the solid due to higher solubility in the liquid phase. This solute redistribution leads to segregations (chemical heterogeneities) at micro-scale, and may lead to macrosegregation, i.e. segregation at larger scale, when coupled with transport phenomena such as thermosolutal convection and solidification shrinkage, see [1] for some details. These macrosegregations are particularly unwanted by ingot producers as they may weaken the mechanical properties of the final piece. Thus, lots of efforts are led to finely understand their origin and control their expansion, with the help of both experimental and modelling studies.



The accurate modelling of macrosegregation phenomena is highly complex as it implies multi-scale and multi-physics problem. Several models are available in the literature, from purely thermal simulations to multi-phase models describing both liquid and solid phase dynamics, see [1] for a review. For instance, recent models include the prediction and description of the solidification structures and their link with macrosegregation, see [2] for instance. A classical in-between approach consists in assuming a motionless solid phase with a mushy zone governed by the Darcy's law. The thermosolutal convection is accounted for through the Boussinesq approximation and a strongly coupled systems of equations is obtained, including momentum, mass and energy conservation equations for the liquid-solid mixture.

In the following, a classical solidification model originally introduced by Benon & Incropera [3] is implemented in the open-source software *Code Saturne* [4, 5] developed by EDF R&D. This software is used for industrial applications and research activities in several fields related to energy production and safety (thermal-hydraulics simulations of incidental situations), process engineering (plasma, electric arcs), gas and coal combustion, turbomachinery, aerodynamics (ventilation, pollutant dispersion). It solves the Navier-Stokes or Reynolds averaged Navier-Stokes equations for 2D, 2D axisymmetric and 3D flows in steady or unsteady, laminar or turbulent, dilatable, incompressible, isothermal cases. The solver is based on a co-located finite volume approach and is highly parallelized. The model and the associated numerical scheme are described first in this paper. Then, the simulated segregation predictions are validated against both academic test case and industrial ingot configurations. A convergence study is also led focusing on time step and mesh size sensitivities.

2. Solidification model

The solidification model presented in this section is a mixture liquid-solid model based on the work of Benon & Incropera [3]. It consists in averaging the local conservation equations of each phase on a Representative Elementary Volume (REV), typically the size of several dendrites, and summing the contributions of both phases to get the mixture dynamics. The volume fraction g_k of each phase in the REV is introduced ($k = l$ stands for the liquid while $k = s$ stands for the solid) such that $g_l + g_s = 1$, and a mixture variable φ is defined as $\varphi = g_l\varphi_l + g_s\varphi_s$. In addition, the following assumptions are considered:

- i. The temperature is in equilibrium between both phases, i.e. the mixture temperature T verifies $T = T_l = T_s$.
- ii. The density is constant and equal in both phases except for the buoyancy force where the Boussinesq approximation is applied; the mixture density ρ verifies $\rho = \rho_l = \rho_s$ and the buoyancy force $\mathbf{F}_b$ writes:

$$\mathbf{F}_b = \rho_b(T, C)\mathbf{g} = \rho \left(1 - \beta_T(T - T_{\text{ref}}) - \beta_C(C - C_{\text{ref}}) \right) \mathbf{g}. \quad (1)$$

- iii. The solid phase is motionless, i.e. the mixture velocity $\mathbf{u}$ verifies $\mathbf{u} = g_l\mathbf{u}_l$.
- iv. The mushy zone is modelled as a porous medium where a drag force $\mathbf{F}_u$ derived from the Darcy's law applies:

$$\mathbf{F}_u = -\frac{\mu_l}{K(g_l)}\mathbf{u}, \quad K(g_l) = \frac{\lambda_2^2}{180} \frac{g_l^3}{(1 - g_l)^2}. \quad (2)$$

The resulting conservation equations governing the mixture dynamics are listed below:

- Mass and momentum conservation equation

$$\begin{cases} \text{div}(\rho\mathbf{u}) = 0, \\ \partial_t(\rho\mathbf{u}) + \text{div}(\rho\mathbf{u} \otimes \mathbf{u}) = -\nabla P + \text{div}(\mu_l \nabla \mathbf{u}) + \rho_b(T, C)\mathbf{g} - \frac{\mu_l}{K(g_l)}\mathbf{u}. \end{cases} \quad (3)$$

- Energy conservation (temperature formulation)

$$c_p(\partial_t(\rho T) + \text{div}(T\rho\mathbf{u})) = \text{div}(\lambda\nabla T) - \partial_t(\rho g_1 L). \quad (4)$$

- Species conservation

$$\partial_t(\rho C) + \text{div}(\rho C_1 \mathbf{u}) = \text{div}(\rho D \nabla C). \quad (5)$$

In order to close the model, the liquidus slope is linearized as:

$$T = T_m + m_1 C_1, \quad (6)$$

and a micro-segregation model is specified. In the following, the lever-rule model is chosen (perfect diffusion in the solid phase), which leads to $C_1 = C/(g_1 + g_s k_p)$ and to the following solidification path:

$$g_1(T, C) = 1 - \frac{1}{1 - k_p} \frac{T - T_1(C)}{T - T_m}. \quad (7)$$

This model offers at least an interesting description of columnar solidification with a limited number of physical parameters to tune, compared to advanced solidification models [2, 6]. It may also be extended to multicomponent alloys adding for each component, a species conservation equation, its buoyancy force contribution and a micro-segregation model. The solidification is modified subsequently integrating all components in the thermodynamic equilibrium.

3. Numerical scheme

The solidification model under consideration displays strong coupling through source terms and includes an incompressible Navier-Stokes system to solve. In practice, it is proposed to solve first the scalar equations for T and C , deduce g_1 and C_1 through closure laws, and finally use a classical SIMPLEC algorithm [7] to handle the velocity-pressure coupling. The scalar fields included in the buoyancy force and the drag force are thus up to date when solving the momentum conservation equation. Sub-iterations are performed to ensure the convergence of the velocity field (10 sub-iterations are chosen in practice), following a PISO-like approach [7].

Denoting n the current time iteration, k the current sub-iteration, and Δt the time step, the time discretization scheme is of order 1 and writes in sequence:

- i. Solve the scalar equations for T and C .

$$\begin{cases} \rho \frac{C^{n+1,k} - C^n}{\Delta t} + \text{div}(C_1^{n+1,k-l} \mathbf{Q}^{n+1,k-l}) = \text{div}(\rho D \nabla C^{n+1,k}), \\ c_p \rho \frac{T^{n+1,k} - T^n}{\Delta t} + c_p \text{div}(T^{n+1,k} \mathbf{Q}^{n+1,k-l}) = \text{div}(\lambda \nabla T^{n+1,k}) - s_T^{n+1,k}, \end{cases} \quad (8)$$

$$\text{where } s_T^{n+1,k} = \partial_T(\rho g_1 L)^{n+1,k-l} \frac{T^{n+1,k} - T^n}{\Delta t} + \partial_C(\rho g_1 L)^{n+1,k-l} \frac{C^{n+1,k} - C^n}{\Delta t}.$$

- ii. Update g_1 and C_1 following the phase diagram: use equations (6) and (7).
- iii. Velocity prediction : ($\mathbf{u}^n \rightarrow \tilde{\mathbf{u}}^k$)

$$\rho \frac{\tilde{\mathbf{u}}^k - \mathbf{u}^n}{\Delta t} + \text{div}(\tilde{\mathbf{u}}^k \otimes \mathbf{Q}^{n+1,k-l}) = -\nabla P^{n+1,k-l} + \text{div}(\mu_1 \nabla \tilde{\mathbf{u}}^k) + \rho_b^{n+1,k-l} \mathbf{g} - \frac{\mu_1}{K^{n+1,k}} \tilde{\mathbf{u}}^k. \quad (9)$$

iv. Pressure correction: ($\tilde{\mathbf{u}}^k \rightarrow \mathbf{u}^{n+1,k}$)

$$\begin{cases} \rho \frac{\mathbf{u}^{n+1,k} - \tilde{\mathbf{u}}^k}{\Delta t} = -\nabla \Phi^k + \delta \rho_b^{n+1,k}, \\ \text{div}(\mathbf{Q}^{n+1,k}) = 0. \end{cases} \quad (10)$$

with:

$$\begin{cases} \delta \rho_b^{n+1,k} = \rho_b^{n+1,k} - \rho_b^{n+1,k-1}, \\ P^{n+1,k} = P^{n+1,k-1} + \Phi^k. \end{cases} \quad (11)$$

The steps i-iv are repeated until, $\|\mathbf{u}^{n+1,k} - \mathbf{u}^{n+1,k-1}\|_{L^2} \leq \epsilon \|\mathbf{u}^n\|_{L^2}$, with $\epsilon = 10^{-5}$. Note that the buoyancy force is also included in the pressure-correction step, which ensure its discrete equilibrium with the pressure gradient. Also, mass fluxes towards solidified cells are not allowed. The spatial discretization is a first-order upwind scheme and note that the variables $\mathbf{u}$, P , T and C are computed at the centre of cells (co-located approach) while the mass fluxes are computed at the faces. As already stated in the introduction of this paper, the *Code_Saturne* open-source software allows to solve this model in a parallel environment with 2D or 3D meshes composed of hexahedron. Numerical results on both academic and industrial configurations are presented in the next section.

4. Simulation results

In this section, two configurations are simulated. The first one is an academic configuration, corresponding to a binary Pb-18%Sn alloy [8], while the second one is an industrial configuration, corresponding to a 3.3 t steel ingot [6].

4.1. Hebditch and Hunt benchmark

This configuration is a numerical benchmark proposed in [8], based on the experiment of Hebditch & Hunt. As presented in figure 1, it corresponds to a rectangular cavity of 0.1 m wide and 0.06 m high. The top and bottom walls are assumed to be adiabatic, while the two vertical walls are cooled (Fourier conditions). For the flow, a non-slip condition is imposed on all the boundaries of the domain. Due to the symmetry of geometry and boundary conditions, and assuming the symmetry of the solution, only half of the domain was considered. At the initial time, the Pb-18%Sn alloy is assumed at rest (no velocity) and its temperature equal to the liquidus temperature corresponding to its nominal composition. The thermophysical properties are identical to the ones used in the literature [8].

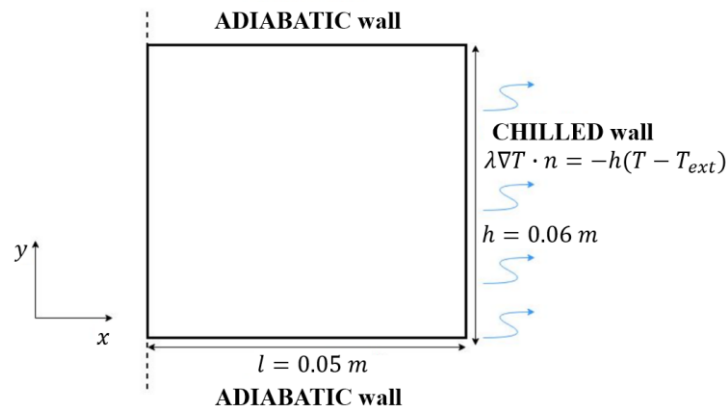


Figure 1. Geometry and boundary conditions for the Hebditch and Hunt benchmark [8].

The resulting segregation map of Sn is presented in figure 2, considering a time step of 10^{-3} s and decreasing the space step from $dx = 1$ mm (3000 cells) to $dx = 0.25$ mm (48000 cells). A comparison is

also proposed with the SOLID[®] software [2, 6, 9], which is based on a 2D finite volume solver and already validated for this configuration [8]. Results obtained by the 2 codes compare well on the finer mesh and the principal characteristics of macrosegregation can be identified: the last part to solidify, i.e. the upper left corner, is positively segregated, while the bottom right is negatively segregated. Segregated channels are also captured with better resolution when refining the mesh. As stated in [8], note that these channels are very sensitive to the mesh size and the numerical method such that no reference solution is currently available in the literature for this test case.

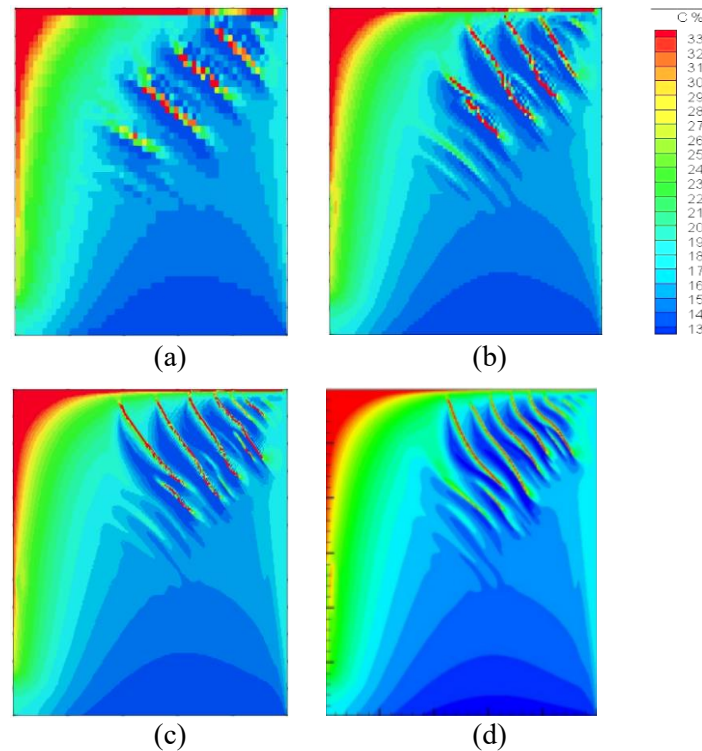


Figure 2. Sn segregation map at the end of solidification: mesh sensitivity with *Code_Saturne* and comparison with SOLID[®]. *Code_Saturne*: (a) $dx = 1$ mm, (b) $dx = 0.5$ mm, (c) $dx = 0.25$ mm, SOLID: (d) $dx = 0.25$ mm.

4.2. Aubert & Duval 3.3 t steel ingot

In this section, a 3.3 t steel ingot configuration described in figure 3 is simulated. The ingot is 2 m in height and 0.6 m in average diameter, and the steel is simplified as a binary Fe-C alloy with a nominal composition of $C_0 = 0.36$ wt%. Heat exchange are modelled within *Code_Saturne*, between the alloy, the mold and the exothermal powder. This configuration being widely studied in the literature for solidification solver validation, please report to [6] for its complete description. As presented on figure 3, the computational domain is 2D axisymmetric with hexahedron cells (7000 cells with $dx = 1$ cm). In the following, the numerical study focuses on time step sensitivity (figure 4) and mesh size sensitivity (figure 5) regarding segregation predictions.

Starting with the time step sensitivity analysis presented on figure 4, the expected segregation pattern is obtained, with a negative segregation cone at the bottom and a positively segregated hot top. Furthermore, some segregated channels are captured just below the hot top and could be referred to as A-segregation [1]. The solution differs notably from $dt = 10^{-2}$ s to $dt = 10^{-3}$ s while the smaller time step offers slight variations around the segregated channels. Thus, the intermediate time step $dt = 10^{-2}$ s seems well adapted for this configuration, as for the previous benchmark.

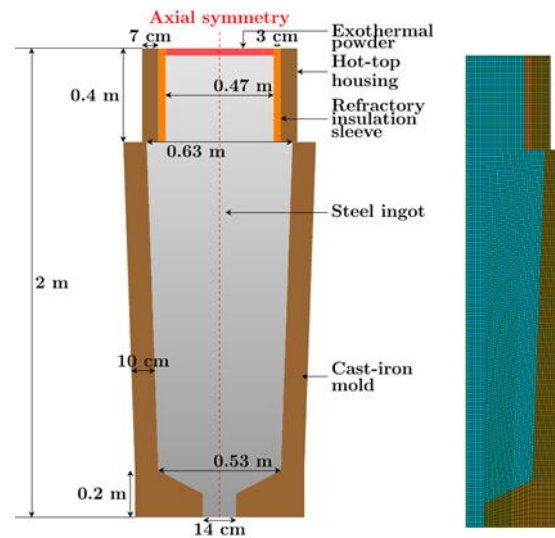


Figure 3. Geometry of the Aubert & Duval 3.3 t steel ingot [6] (left) and computational domain (right).

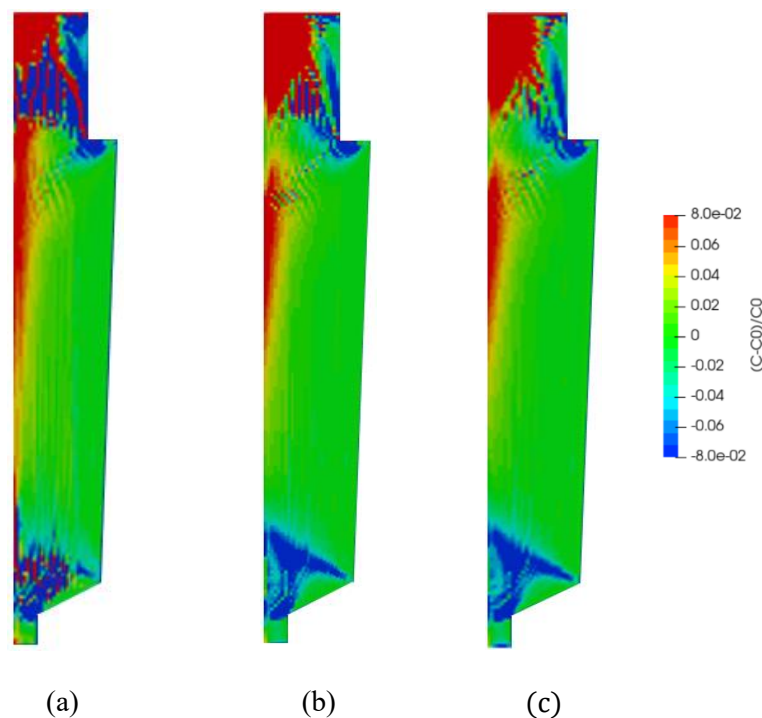


Figure 4. Carbon segregation map: time step sensitivity for a 3.3 t steel ingot ($dx = 1$ cm).
(a) $dt = 10^{-2}$ s, (b) $dt = 10^{-3}$ s, (c) $dt = 10^{-4}$ s.

Regarding the mesh sensitivity analysis on figure 5, ranging from 2000 cells ($dx = 2$ cm) to 30000 cells ($dx = 0.5$ cm), the main segregation patterns seem already well captured with the intermediate mesh composed by 7000 cells ($dx = 1$ cm). The finer mesh still yields different results when focusing on segregated channels. From these observations, it seems difficult to conclude about the physical and/or numerical origin of these channels; further numerical and experimental validation have to be conducted in that sense. At the end, the intermediate time step combined with the intermediate mesh seems to offer a reasonable compromise.

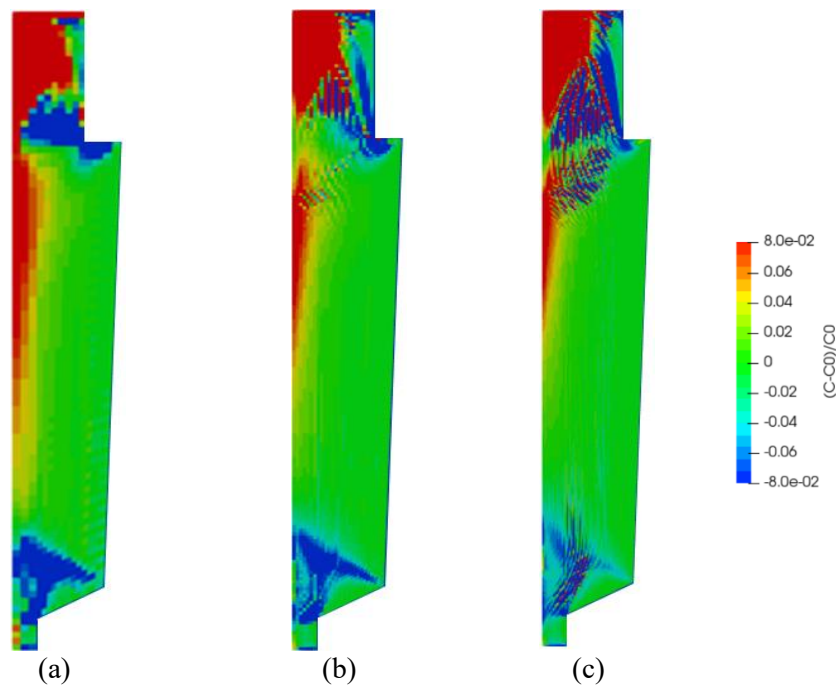


Figure 5. Carbon segregation map: mesh size sensitivity for a 3.3 t steel ingot ($dt = 10^{-3}$ s).
(a) $dx = 2$ cm, (b) $dx = 1$ cm, (c) $dx = 0.5$ cm.

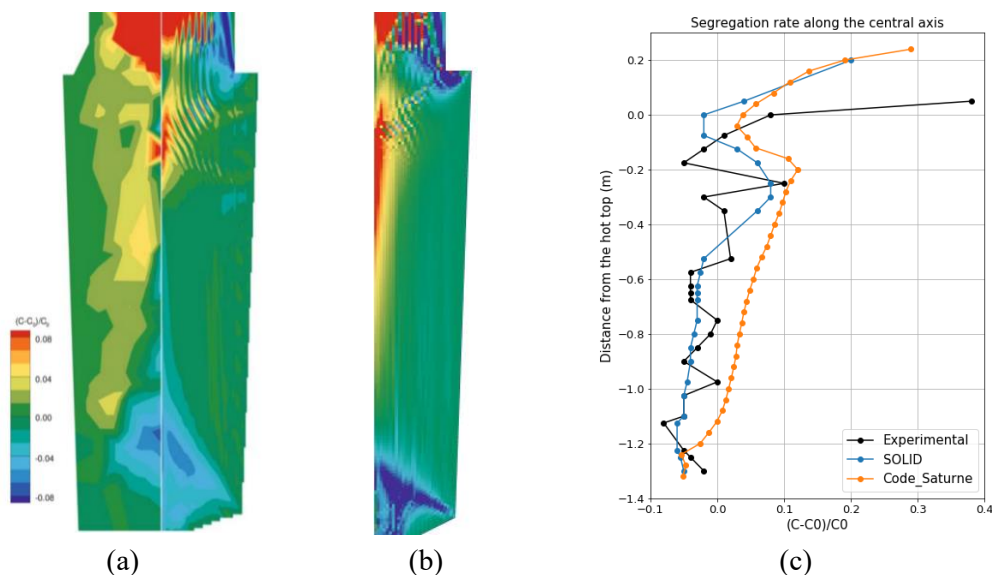


Figure 6. Comparison between experimental data, SOLID[®] and *Code_Saturne* results for a 3.3 t ingot. (a) Experimental (left) and SOLID results (right), (b) *Code_Saturne* results, (c) Axis segregation rate.

On figure 6, the segregation results are compared with the SOLID[®] and experimental results. Correct agreement is found between the 2 codes which are able to capture the main trends of the experimental data. However, note that the large positive segregation zone aside the central axis, which extends from the hot top to the negative segregation cone (in yellow on the experimental map), is not captured numerically. It might result from a non-modelled physical phenomena, such as the movement and sedimentation of equiaxed grains coming from nucleation or dendritic fragmentation, see [2] for instance.

5. Conclusion

This paper presents a solidification model with an associated numerical scheme implemented in the open-source software *Code_Saturne*. This model is a classical liquid-solid mixture model which accounts for thermosolutal convection and assumes a motionless solid phase. The numerical results are comparable with similar approaches available in the literature, offering mainly qualitative prediction of segregations. These results also highlight the difficulties to obtain converged results when focusing on segregated channels. Further development are conducted in that sense in *Code_Saturne* with the aim of improving the accuracy and the efficiency of numerical methods for solidification models.

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Nomenclature

β_T	Thermal expansion coefficient (K^{-1})	k_p	Partition coefficient
β_C	Solutal expansion coefficient (K^{-1})	P	Pressure (Pa)
C	Bulk Concentration (wt. pct.)	Q	$\rho \mathbf{u}$ ($kg.m^{-2}.s^{-1}$)
C_k	Liquid or solid concentration	ρ	Density ($kg.m^{-3}$)
c_p	Specific heat per unit mass ($J.kg^{-1}.K^{-1}$)	ρ_b	Boussinesq density ($kg.m^{-3}$)
D	Diffusion coefficient ($m^2.s^{-1}$)	μ_l	Dynamic viscosity of the liquid (Pa.s)
Δt	Time step (s)	T	Temperature (K)
g	Gravity acceleration ($m.s^{-2}$)	T_l	Liquidus temperature (K)
K	Permeability (m^2)	T_m	Melting temperature (K)
L	Latent heat ($J.kg^{-1}$)	$\mathbf{u}$	Velocity ($m.s^{-1}$)
λ	Thermal conductivity ($W.m^{-1}.K^{-1}$)	g_k	Volume fraction of phase k
λ_2	Secondary Dendritic Arm Space (m)	l,s	Subscript referring to liquid and solid phase
m_l	Liquidus slope (K/wt.pct.)	ref	Subscript referring to reference value

References

- [1] Pickering E J 2013 *ISIJ int.* **53** 935
- [2] Gerin B, Combeau H, Založnik M, Poitraul I and Cherif M 2019 *Proc. IOP Conf. Ser. Mater. Sci. Eng.* **529** 012036
- [3] Bennon W D and Incropera F P 1987 *Int. J. Heat Mass Trans.* **30** 2161
- [4] <https://www.code-saturne.org>
- [5] Archambeau F, Méchitoua N and Sakiz M 2004 *Int. J. Finite Vol.* **1** 1
- [6] Combeau H, Založnik M, Hans S and Richy P E 2009 *Metall. mater. trans. B* **40** 289
- [7] Versteeg H K and Malalasekera W 2007 *An introduction to computational fluid dynamics: the finite volume method* (Pearson education)
- [8] Combeau H *et al.* 2012 *Proc. IOP Conf. Ser. Mater. Sci. Eng.* **33** 012086
- [9] Ahmad N, Combeau H, Desbiolles J L, Jalanti T, Lesoult G, Rappaz J, Rappaz M and Stomp C 2017 *Metall. Mater. Trans. A* **29** 617