Modelling of Macrosegregation in Continuous Casting of Aluminium

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Abstract

Within the framework of the Brite-Euram research program EMPACT (A European Modelling Programme on Aluminium Casting Technology), macrosegregation in continuously cast Al-Mg slabs has been modelled. For that purpose, the average conservation equations of mass, momentum, heat and solute were derived, including the shrinkage contribution and the transport of the solid. Solvers for these equations were implemented in the Finite Element software calcoMOS. At each time step, the variations of enthalpy and average solute contents were computed by successive solution of the above equations. A microsegregation model then allowed to determine the increments of the volume fraction of solid, temperature, liquid and solid concentrations, and average density. This model encompassed back-diffusion in the primary phase and non-linear phase diagrams. It was found that the negative and positive segregations measured at the centre and surface of DC cast ingots, respectively, could be explained to a fairly large extent by the solidification shrinkage contribution.

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1. Introduction

Unlike microsegregation which can be modified by subsequent heat treatments, *macrosegregation*, i.e., alloy composition heterogeneity at the scale of a whole casting, remains during the various treatments applied to DC cast ingots (rolling, homogenisation, etc.). Therefore, it is essential to control it and simulation is a means of achieving that.

Macrosegregation is the result of the coupling of two phenomena : *microsegregation* at the scale of the dendrites and *relative movement* between the solid and liquid phases at the scale of the casting [1]. The relative movement between the solid and liquid phases can be induced by : natural or forced convection, solidification shrinkage, sedimentation of equiaxed grains or deformation of the mushy zone [1].

In the present calculations, only the first two mechanisms were taken into account. The model has therefore to solve first the heat flow equation in order to predict the location of the mushy zone and the enthalpy field (see Fig. 1). Second, the movement of the liquid phase is calculated with the help of the momentum and mass conservation equations. Finally, the solution of the average solute concentration equation(s) gives the evolution of the average solute content at any location. These last equations must be coupled with a microsegregation model, which allows to calculate the solidification path at every location.

The calcoMOS Finite Element (FEM) software [2], which simulates solidification phenomena for two-dimensional (2D) cartesian and axisymmetric geometry, was used to implement macrosegregation computations. This paper briefly presents the model and its application to DC cast aluminium ingots.

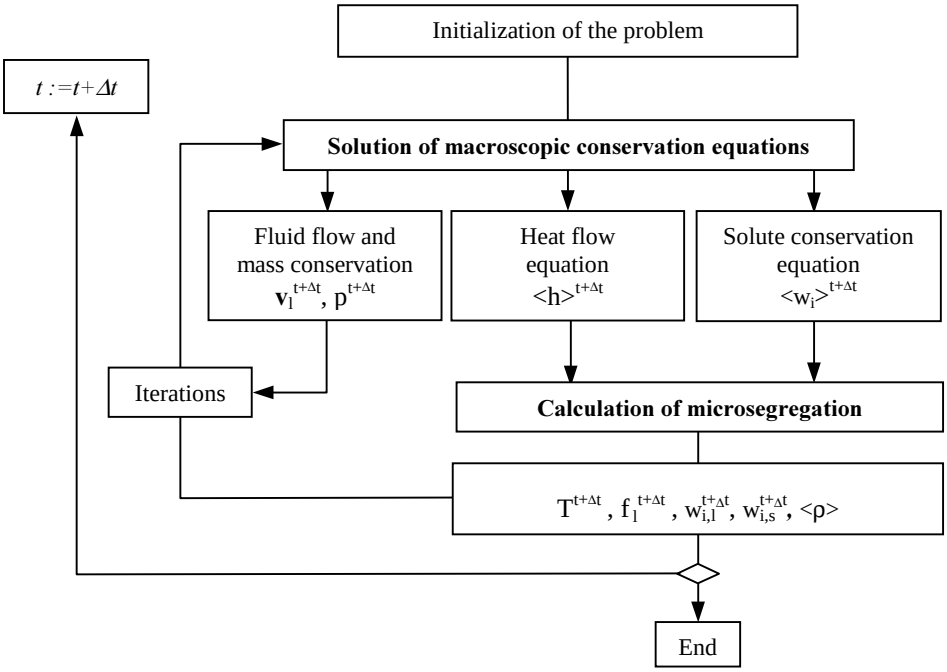


Figure 1 : *Flow chart of the macrosegregation computation.*

2. Model Description

In the presence of shrinkage and solid transport at a uniform velocity, $\mathbf{v}_s$, the average conservation equations for heat, mass and solute species are given by [3]:

$$\text{Heat :} \qquad \frac{\partial \langle \rho h \rangle}{\partial t} + \text{div} \langle \rho h \mathbf{v} \rangle - \text{div} (\langle \kappa \rangle \, \mathbf{grad}\, T) = 0 \qquad (1)$$

$$\text{Mass :} \qquad \frac{\partial \langle \rho \rangle}{\partial t} + \text{div} \langle \rho \mathbf{v} \rangle = 0 \qquad (2)$$

Solute (i) : $$\frac{\partial <\rho w_i>}{\partial t} + \text{div} <\rho \mathbf{v} w_i> = 0 \qquad (3)$$

where $<\xi>$ denotes the average over the liquid and solid phases of the field ξ, i.e., $<\xi> = \xi_s g_s + \xi_l g_l$, where ξ_s and ξ_l are the values in the solid and liquid phases, g_s and g_l being the volume fractions of solid of liquid, respectively. ρ is the specific mass, h is the enthalpy per unit mass, $\mathbf{v}$ is the velocity, κ is the thermal conductivity, T is the temperature and w_i is the mass fraction of solute species (i). For this last entity, the local averaging of the solute concentration, $<\rho w_i>$, is slightly different if microsegregation does not occur at equilibrium (i.e., not according to lever rule) :

$$<\rho w_i> = \rho_l w_{i,l} g_l + \int_0^{g_s} \rho_s w_{i,s}(g,t) dg \qquad i = 1, N \qquad (4)$$

where N is the number of solute species.

The momentum conservation equation is usually written only for the liquid phase. In the case of global transport of the solid, such as that encountered in DC casting, this can be done for the relative velocity of the fluid $\mathbf{u} = (\mathbf{v} - \mathbf{v}_s) = (\mathbf{v}_s g_s + \mathbf{v}_l g_l) - \mathbf{v}_s = g_l(\mathbf{v}_l - \mathbf{v}_s)$. One has :

$$\rho_l \frac{\partial \mathbf{u}}{\partial t} + \frac{\rho_l}{g_l} (\mathbf{Grad\ u}) \cdot \mathbf{u} - \mu \Delta \mathbf{u} + \frac{\mu g_l}{K} \mathbf{u} + g_l \mathbf{grad}\ p = g_l \rho_b \mathbf{g} \qquad (5)$$

μ is the dynamic viscosity of the fluid, K the permeability of the mushy zone and ρ_b the Boussinesq approximation of the density of the fluid :

$$\rho_b = \rho_{l,o} [1 - \beta_T (T - T_o) - \sum_i \beta_i (w_{i,l} - w_{i,l,o})] \qquad (6)$$

$\rho_{l,o}$ is a nominal specific mass of the liquid taken at some reference temperature, T_o, and concentrations in the liquid, $w_{i,l,o}$. β_T and β_i are the thermal and solutal expansion coefficients, respectively.

The schematic flowchart of the program is given in Fig. 1. Without giving the details of the formulation which can be found in [3], these equations are solved at the scale of the whole casting as follows :

1. The heat flow conservation equation is solved according to an enthalpy scheme [2], i.e., using the enthalpy as the variable and linearising the temperature-enthalpy relationship. The velocity field of the previous time step is used.
2. The mass and momentum conservation equations are solved simultaneously using a GLS (Galerkin Least Squares) formulation for the pressure-velocity fields [4]. The temperature, volume fractions, solute concentrations and variations of the average specific mass (shrinkage) are taken from the previous time step.
3. Once the relative velocity of the fluid is known, the solute conservation equation(s) are solved in order to deduce the new average solute concentrations.

Knowing the average enthalpy, $<h>^{t+\Delta t}$, and solute concentrations, $<w_i>^{t+\Delta t}$, at all the nodes of the mesh, the new temperature, volume fractions of phases, solute concentrations in the liquid and solid phases, and average specific mass are calculated according to a local microsegregation model. In the present case, the model developed by H. Combeau and A. Mo for binary alloys has been used [5]. It allows to consider non-linear phase diagrams, eutectic reaction and back-diffusion. It should be pointed out that the ternary model developed by X. Doré within the framework of this project [6] for Al-Mg-Si alloys has also been implemented in calcoMOS.

The microsegregation model is equivalent to solving at each nodal point the N equations (4) with the following ones [5,6]:

Equilibrium at the interface : $$w^*_{i,s} = k_i w_{i,l} \qquad i = 1, N \qquad (7)$$

Liquidus relationship : $$T = T_L(w_{i,l}) \qquad (8)$$

Enthalpy relationship : $$<\rho h> = <\rho c_p> T + <\rho> L g_l \qquad (9)$$

The k_i's are the partition coefficients, T_L is the equation of the liquidus, $<\rho c_p>$ is the average volumetric specific heat and L is the latent heat of fusion. When precipitation of secondary phases occurs, the problem becomes more complex and is not detailed here [5,6]. Providing a back-diffusion model is given (i.e., evolution of $w_{i,s}(g,t)$ appearing in Eq. (4)), Eqs. (4,7-9) provide (2N + 2) equations for the (2N + 2) unknowns : $w_{i,s}$, $w_{i,l}$, T and g_l.

This back-diffusion model can be given either by a polynomial function approximation of $w_{i,s}(g,t)$ [5] or by the solution of Fick's second law in the solid phase using a 1D FDM technique [6].
In the case of DC casting of Al alloys in which one is interested mainly in the stationary solution, the time stepping is used as a means of iteration among the equations. In this case, however, the Eulerian description of the macroscopic conservation equations (i.e., in a reference frame attached to the mould) must be coupled with a Lagrangian description of microsegregation (i.e., in a reference frame attached to the dendrites). Details of this coupling can be found in [3].

Results

The results which are presented in this section are for an Al-Mg alloy, using the microsegregation model of [5]. Fig. 2 shows the calculated stationary 2D velocity field near the liquidus isoline for a small DC cast ingot 5-cm thick. For symmetry reason, only half the ingot has been calculated over a length of 15 cm. The metal was supposed to be injected uniformly from the top at a velocity of 1 mms^{-1} with a nominal concentration of 4.5% Mg. Three calculations were performed under identical conditions but considering various sources of fluid movement : buoyancy only (case (a)), shrinkage only (case (b)) and buoyancy plus shrinkage (case (c))
As can be seen, the relative velocity of the fluid in the fully liquid region (i.e., above the first isoline of fraction of solid also represented in this figure) is of the order of cms^{-1}, regardless of whether shrinkage is included or not in the calculations (compare Figs. 2a and 2c). It is induced by thermal buoyancy, the solutal expansion coefficient associated with magnesium being small. Despite this fairly large relative velocity of the liquid, the induced macrosegregation is almost negligible when only buoyancy is considered (see Fig. 3). This is due to the fact that the flow pattern in this case is essentially parallel to the liquidus isotherm, i.e., perpendicular to the solute gradient, and vanishes quickly in the mushy zone.

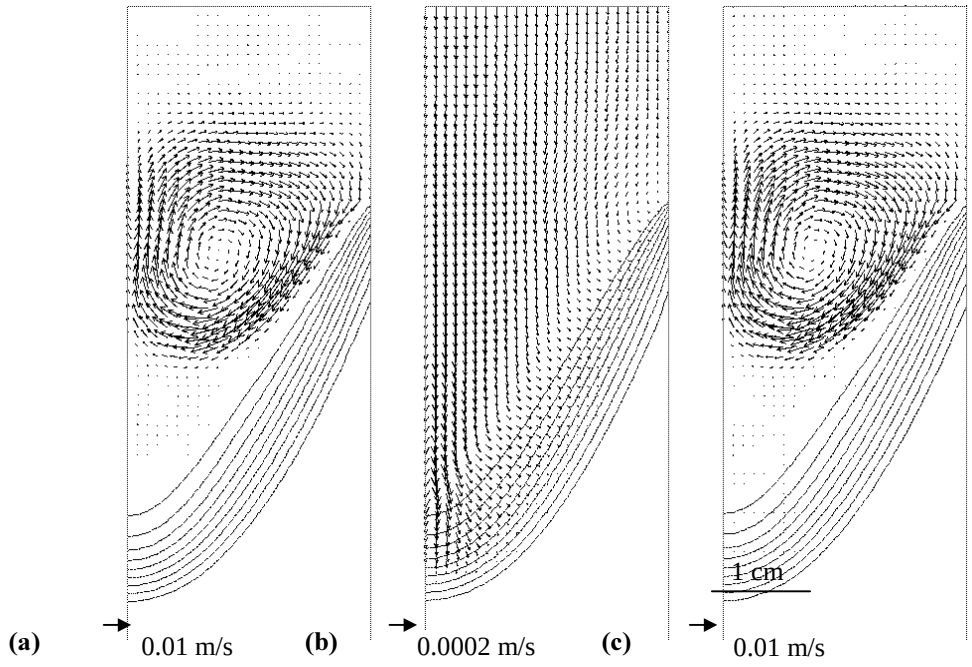


Figure 2 : *Calculated stationary field of the relative fluid flow velocity for a small DC cast Al-4.5%Mg ingot (casting speed : 1 mms^{-1}) with isolines of fraction of solid. a) buoyancy only ; b) shrinkage only ; c) buoyancy and shrinkage. Microsegregation model of Ref. [5] with a Scheil approximation.*

As reviewed in [1] and pointed out many years ago by Flemings, it is the component of the velocity along the thermal gradient which induces macrosegregation. Although the shrinkage-induced velocity is nearly two orders of magnitude smaller than that associated with thermal buoyancy (see Fig. 2b), it has a much more pronounced influence on the final concentration profile at the exit of the ingot (Fig. 3). In the mushy zone, the relative velocity of the fluid is on the order of 0.2 mms^{-1} only, but it is nearly perpendicular to the isofractions of solid. (Please note that the same flow exists in the mushy zone of Fig. 2c but is not visible with the scale used to visualise the overall flow pattern). Since the streamlines of the interdendritic fluid flow deviate from the ingot centerline (Fig. 2b), this induces a negative segregation at the center of the ingot and a positive one at the surface

(Fig. 3). This shrinkage-induced segregation, commonly labeled “inverse segregation” in static castings [1], increases with the depth of the liquid pool, i.e., with the casting speed [3].

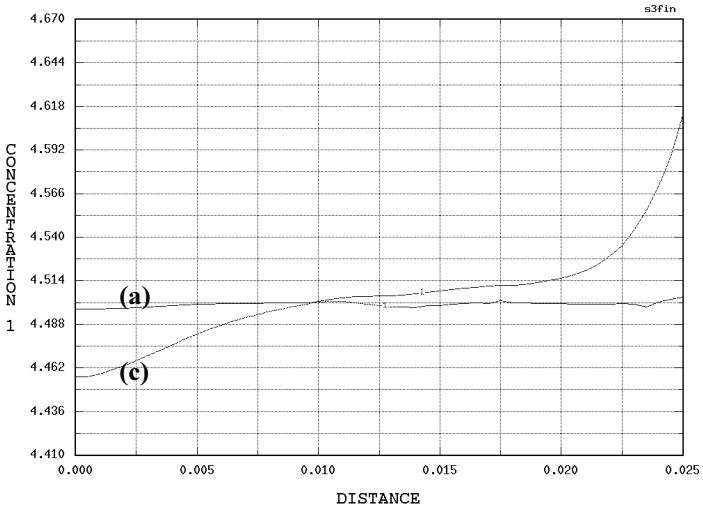
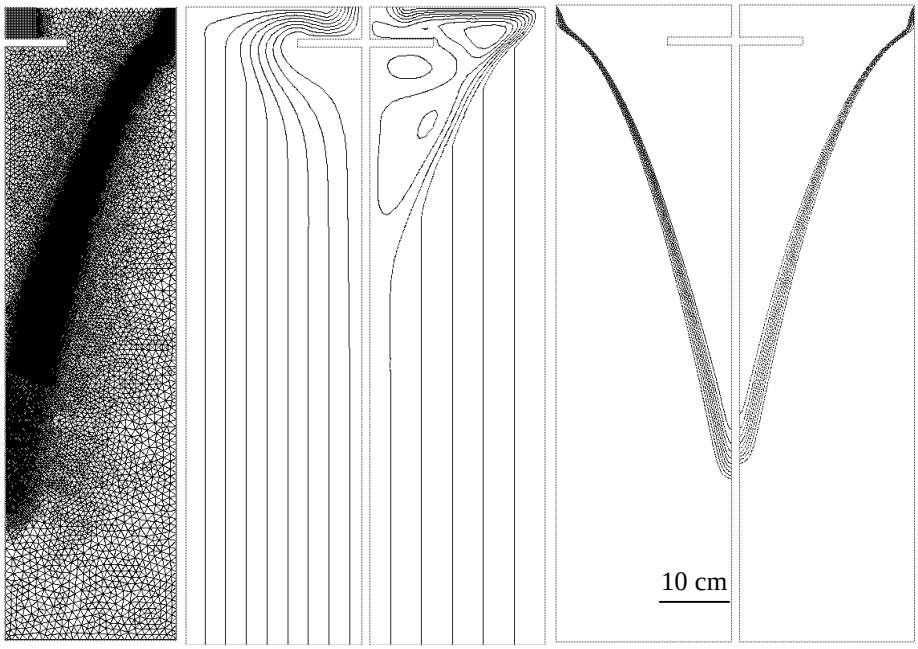


Figure 3 : *Mg concentration profiles at the exit of the small DC cast ingot for the cases involving buoyancy only (a) and buoyancy plus shrinkage (c) of Fig. 2.*

The same phenomenon can be observed in real-size ingot computations (Figs. 4 and 5). Unlike small DC castings for which a good resolution can be obtained with a structured mesh following the coordinate axes [3], large scale simulations have to be performed with an unstructured mesh in order to obtain a sufficient accuracy within a reasonable CPU time. A first thermal calculation allowed to determine the approximate position of the mushy zone in this 0.25×1 m^2 domain and to refine the mesh in this region (Fig. 4a). Feeding of metal through a distribution bag was simulated by inserting a horizontal plate inside the domain. Since the Eulerian-Lagrangian algorithm implemented in calcoMOS for back-diffusion calculations requires, at present, structured meshes (i.e., mesh points aligned along verticals), the macrosegregation result shown in Fig. 5 was obtained with the lever-rule approximation.

In Fig. 4, the streamlines and isolines of fraction of solid are shown for the two cases of shrinkage only (case (a)) and shrinkage plus buoyancy (case (b)). In the first case (Fig. 4(2a)), the streamlines turn around the horizontal plate and then are fairly straight : they directly outline feeding of the ingot from the upper gate to the mushy zone. On the contrary, thermal buoyancy in the liquid pool is turbulent if a laminar viscosity value is used : it gives rise to a complex fluid flow pattern, which never reaches a stationary state. Since no turbulent model was implemented in calcoMOS, an artificially increased viscosity by a factor 100 was used to obtain the result shown in Fig 4(2b). Results obtained with such an increased-viscosity approximation have been compared recently with those calculated with a turbulent model [7].

One can notice the influence of the primary and secondary coolings on the isolines of fraction of solid (small cusp near the top of Fig. 4(3)). The corresponding values of the heat transfer coefficients were deduced from experimental measurements and inverse method [8]. As can be seen, thermal buoyancy slighltly modifies the depth of the molten pool. However, the two corresponding segregation profiles at the exit of the ingot calculated for this real-size casting (Fig. 5) do not differ much, thus indicating again that shrinkage-induced macrosegregation is dominant over that associated with natural convection. A negative centerline segregration is again predicted by the simulation. The amount of segregation predicted by this model compares fairly well with the concentrations measured within the framework of the EMPACT project [9].



(1) (2a) (2b) (3a) (3b)

Figure 4 : *Real size DC casting simulation for an Al-4.06%Mg alloy solidified at 1 mms^{-1} : Mesh size (1), velocity streamlines (2) and isolines of fraction of solid (3) for the cases with shrinkage only (a) and with buoyancy plus shrinkage (b). Microsegregation module of [5] used with the lever rule. 16417 nodes, about 24h CPU on SGI2000.*

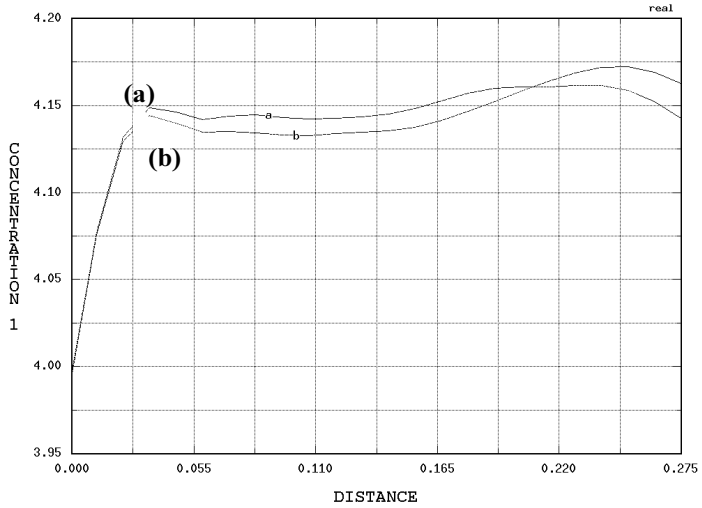


Figure 5 : *Calculated Mg concentration pofiles at the exit of the real-size DC cast Al-4.06%Mg ingot (Fig. 4) for the cases with shrinkage only (a) and with buoyancy plus shrinkage (b).*

Conclusion

Computation of macrosegregation in real-size DC cast ingots is a real challenge, even in two dimensions. The size of the region where both the fluid flow and solute gradients are non-zero is very small compared with the overall size of the ingot. Unstructured meshes offer clearly an advantage in this respect, but they are also more complicated to implement (e.g., for a mixed Lagrangian-Eulerian description). It has been shown in the present contribution that shrinkage-induced macrosegregation can already account for a fairly large portion of the concentration inhomogeneity measured in Al-Mg ingots. Thermal buoyancy has a minor influence for this alloy. This does of course not preclude anything about the influence of other phenomena such as grain movement, deformation of the mushy zone or solutal convection induced by other alloying elements.

Acknowledgements

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