State-of-the-Art in the Modelling of Aluminium and Copper Continuous Casting Processes

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Abstract

With the advent of powerful and cheap computers, modelling of solidification processes at the macroscopic scale has become a standard practice in industry, in particular in continuous casting processes. Indeed, commercial software packages are available for the modelling of heat and fluid flow, as well as for stress-strain calculations. Such software can even be used in an “inverse way” in order to deduce casting parameters (e.g., heat transfer coefficients) from measurements (e.g., temperature). Electro-magnetic stirring, which is increasingly used to refine grain structures, can also be modelled by coupling hydromagnetic and thermal aspects. In more advanced approaches, convection in the liquid, heat exchange and stress developments are coupled all together in a mixed Lagrangian-Eulerian formulation. The start-up phase, which is crucial for many continuous casting processes (e.g., DC casting of Al alloys), is another field of development for which mixed formulation is promise full. Modelling of macrosegregation is still a critical issue as it can have different origins: convection, solidification shrinkage, grain movement/sedimentation, deformation of the mushy zone. Substantial progresses have been made in this area as well. Besides macroscopic aspects, modelling of microstructure and defect formation is an active field of research, in particular for microporosity and hot tearing. The present contribution will review the state-of-the-art modelling of aluminium and copper semi-continuous or continuous casting processes, at both the industrial, more macroscopic, approach and the still more academic, microscopic, level. This review is based on the communication given by M. Rappaz at the occasion of the 40th anniversary of the R&D Centre of Hydro-Aluminium (formely VAW) in Bonn in May 2004 [1].

1 Introduction

From an academic point of view, the VDC (vertical direct chill) casting process is schematically shown in Fig. 1. Although fairly simple in its principle, it involves several interplaying phenomena which finally render modelling approaches complex. At the macroscopic scale (topics 1 to 4), heat and fluid flow modelling is of course the first step in order to predict the delivery of metal, the melt pool depth, the thermal gradient, the local solidification rate, etc ... Fluid flow is also essential in determining macrosegregation, i.e., transport of solute species at the macroscopic scale, and grain structure, i.e., influence of convection on dendrite fragmentation and grain transport. Almost as important is the calculation of stress build-up and strains, since this conditions air gap formation between the ingot and the mould or bottom block, and thus heat transfer. Knowing the deformation of the slabs also helps to calculate the mould shape that will minimise scalping operations, while stress assessment is a key element to predict hot cracking formation.

Although fluid flow and solid deformation are governed by the same basic conservation equations (conservation of mass and momentum), their associated rheologies are so different that combined Eulerian/Lagrangian approaches are required to handle the large displacements/small stresses of the fluid and the small displacement/large stresses of the solid. Although several softwares can now calculate in a coupled way these two aspects, the approaches usually remain "one-phase". If such approaches are very useful in predicting the combined interaction between heat flow, fluid flow and solid deformation, they cannot address in details phenomena occurring in the mushy zone. Recently, one has seen the emergence of "two-phase" approaches in which the solid and liquid equations are averaged over a typical volume element, with appropriate exchange terms, in order to predict hot cracking tendency.

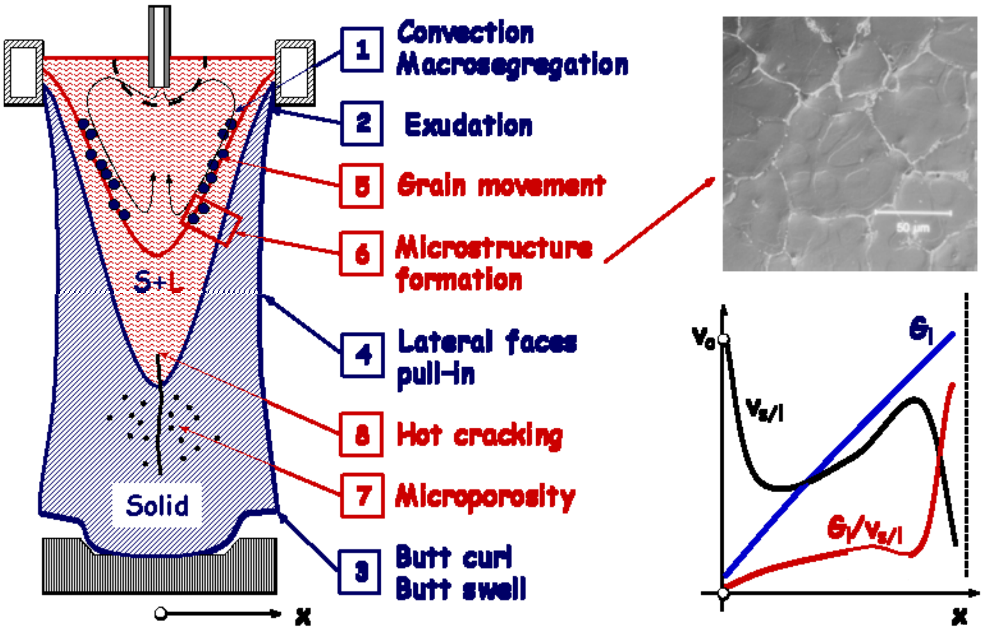

Figure 1: Schematics of the VDC casting process. Topics 1-4 correspond typically to a macroscopic approach, whereas topics 5-8 correspond to a microscopic one. Typical variations of the thermal gradient, G, of the solidification rate, v, and of G/v are shown as a function of x [1].

For a metallurgist, macroscopic entities such as cooling rate, residual stresses, etc., are fine… but not sufficient! He wants to have access to macro- and microstructures as well as to defects such as microporosity and hot cracking (topics 5 to 8 in Fig. 1). While Cellular Automata or granular-type approaches in the mid-nineties were a step forward for the prediction of grain structure formation, the advent at the same time of the phase field method in the materials science community gave great hopes to solve the problem of microstructure prediction. Amazing progresses have been made, but the technique still remain delicate to use and very CPU-intensive. For the prediction of microporosity, one has seen recently the emergence of 3D computations combining solidification shrinkage, gas segregation, nucleation and growth of pores. Finally, the prediction of hot tearing has really become a …. "hot" topic since the first approach combining strains of the solid skeleton and liquid feeding was published in 1999. The present paper reviews very briefly the state of the art of solidification modelling, focusing mainly on DC casting, and will outline some of the challenges that remain. It is largely inspired by the work carried out in two European research projects, EMPACT (1996-2000) and VIRCAST (2000-2004) and in the on-going project POST (Porosity Stress).

2 Macroscopic Modelling

2.1 Heat flow

Heat extraction is of course essential in solidification modelling, not only at the process scale, but also at the level of the microstructure-defects. The thermal gradient, G, and solidification rate, v, can be used in microstructure maps [2]: the fineness of the microstructure is essentially a function of (Gv), i.e., of the cooling rate, while the type of microstructure (e.g., columnar, equiaxed) depends on G/v. Niyama's criterion for microporosity prediction is also a function of G/v [3]. It should be pointed out that, even in the steady state regime, the solidification rate v at the liquidus position depends on position and is not equal to the casting speed, v_c, as shown in Fig. 1. Modelling of heat flow in DC casting is no longer a challenge from a numerical point of view, in the start-up or steady state phases. The enthalpy method with evolving/activated meshes is robust in handling the strong non-linearity associated with latent heat release. The main questions in this area are related to materials properties and boundary conditions. For both, inverse methods have become a standard practice to calibrate the calculations [4]. As an example, Fig. 2 shows the heat flux deduced at the surface of a DC cast ingot as a function of the distance from the top liquid surface. One can clearly distinguish the heat flux associated with primary cooling, the air gap formation (nil flux) and the strong heat extraction associated with water cooling.

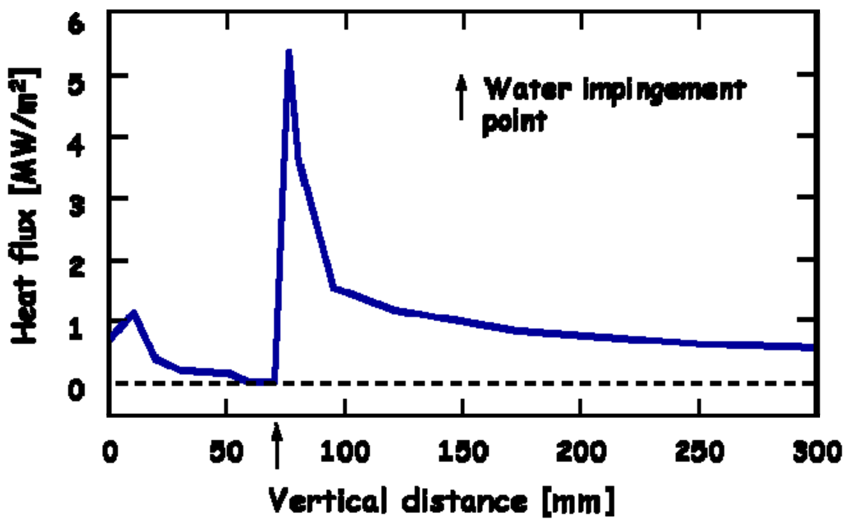

Figure 2: Computed heat flux as a function of the distance to the top liquid level for an AA5182 alloy [4].

2.2 Fluid flow

Despite the advanced CFD (computational fluid dynamics) software on the market, fluid flow calculations remain a task of specialists, especially when solidification occurs simultaneously. Since such calculations are performed in a single domain, containing the liquid and solid phases, a penalty method is used to make the velocity in the solid resume to the casting speed. The viscosity can be made a function of the volume fraction of solid or, better, a drag term similar to Darcy's equation for a porous medium can be introduced in the momentum conservation equation. On the other hand, as the laminar viscosity of metals is very low, a turbulence model is also required to get realistic fluid flow pattern and intensity. One of the challenges that remain in this field is the validation of the calculated velocity field. Although some probes were designed by Vives [5], one has very often to rely on water models to calibrate the flow [6-7]. Another challenge is the interaction between the flow and the mushy zone. Besides fragmentation of dendrites [8] and formation of feathery grains [9,10], which are both favoured by convection, it is not easy to model accurately the narrow boundary layer near the liquidus in a transient regime, since it moves over time and normally requires adaptive-evolving meshes. As an example, Fig. 3 shows the velocity field calculated with Fidap in a round billet fed from the lateral side [10]. The maximum shear rate of the liquid occurs at the opposite side of the gating and favours the growth of twinned dendrites in this region.

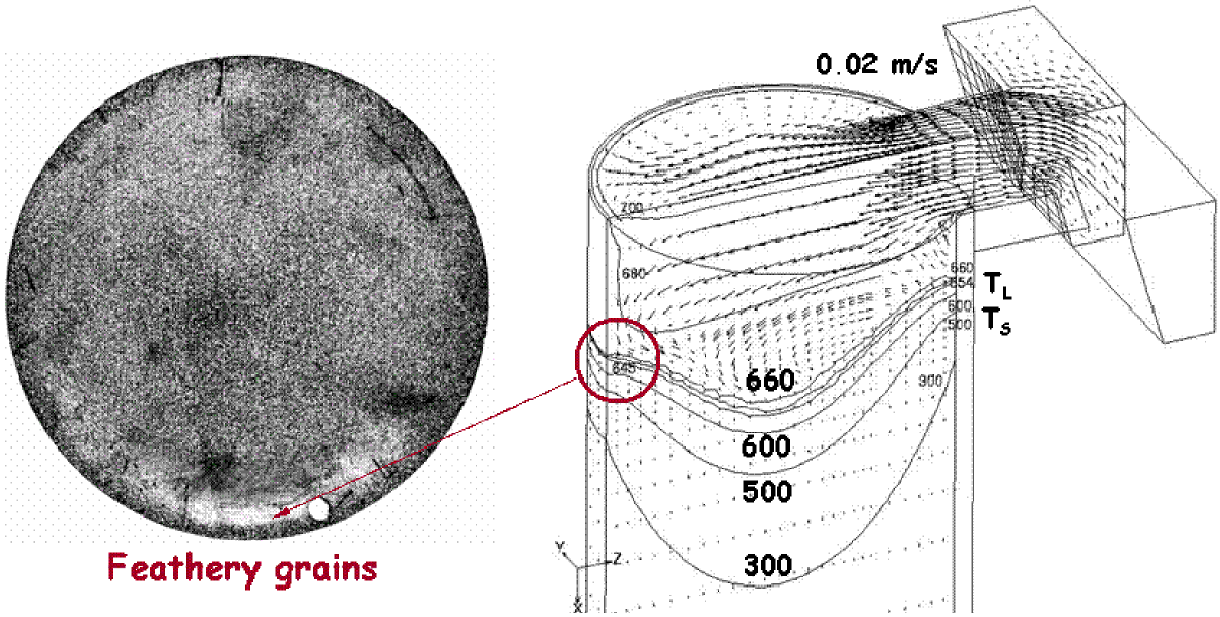

Figure 3: Velocities and temperatures at the surface and in the vertical symmetry-plane for an AA1050 DC cast billet, injected from the lateral side, as calculated with the Fidap software. Temperatures are in °C, (T_{liq} = 657 °C, T_{sol} = 645 °C). In-flow velocity is 0.02 m/s, from [10].

2.3 Stresses and strains

Deformations of the solid during cooling and stress build-up are important issues in DC casting of aluminium alloy [11-13]. Deformation both limits the heat exchange with the mould and bottom block, and thus the production rate, and modifies the shape of the ingot. As shown schematically in Fig. 1, butt curl, butt swell and lateral faces pull-in make the final shape of the slab to deviate from a parallelepipedon. In a transverse section as well, a convex mould has to be used if a rectangular cross section at the end of solidification is desired, since pull-in at the corners is smaller than at the mid-rolling faces. Stresses are also important as they induce hot cracking or even “cold” cracking.

In this area, modelling is very mature, partially thanks to the EMPACT program, and many commercial software exist. However, deformation especially of the lateral faces is strongly influenced by the inclination of the thermal gradient, and thus by the sump shape. For example, an increase of the casting speed makes the liquid sump deeper and thus the thermal gradient more horizontal, in which case pull-in is increased. By the same argument, the shape of the liquid pool being influenced by convection, and therefore by the distribution bag, accurate solid deformation calculations require to couple them, not only with heat-, but also with fluid-flow simulation. This challenge is not met by all commercial software. By the same argument, compressive stresses of the mushy zone can expulse interdendritic liquid out (i.e., sponge effect [14]) thus leading to deformation-induced segregation. Tensile stresses on the contrary lead to an opening of the mushy zone, inducing either segregation (healed hot tears) or hot cracks.

2.4 Macrosegregation

Despite the effort done during the EMPACT program, macrosegregation, i.e., solute inhomogeneity at the scale of the ingot, still remains a challenge in DC casting for several reasons [15]. First, macrosegregation can be induced by solidification shrinkage (inverse segregation) and exudations, by forced or natural convection, by grain movement and sedimentation and by deformation of the solid skeleton in the mushy zone. These effects have been addressed separately, sometimes in a combined approach (e.g., shrinkage and deformation [14] or shrinkage and natural convection [16]), but never in a comprehensive model. Second, each of this topic is complex. For example, deformation-induced segregation requires to couple stress-strain calculation, including the mushy zone, with heat-, mass- and solute-transport in the liquid phase [14]. Third, some of these phenomena are very localized. For segregation induced by natural convection, the origin is the region where both the liquid velocity and the solute gradients are non-zero. It is limited to a region of maybe 1 mm thickness at most near the liquidus surface [16,17].

Nonetheless, some interesting attempts to model macrosegregation have been made. For example, a result obtained in a 2D section of a DC cast slab of an AA5182 alloy is shown in Figure 4 [16]. It has been computed with the software CalcoSOFT, considering shrinkage and natural convection. The main contribution to macrosegregation in this case was found to be due to shrinkage: it induces a negative segregation zone near the centre of the ingot, the magnitude of which corresponds to concentration profile measurements.

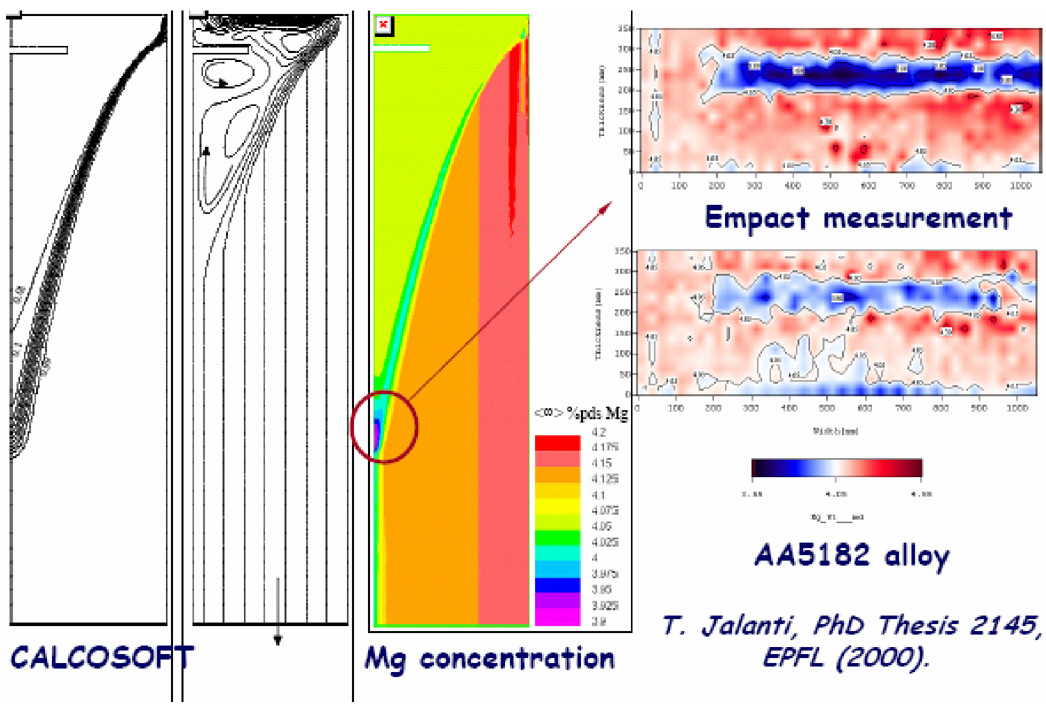

Figure 4: Macrosegregation results for a 2D section of an AA5182 DC cast slab, as calculated with the CalcoSOFT software. The various pictures represent, from left to right: the steady state temperature profile, the iso-fractions of solid showing clearly the mushy zone position, the velocity field, the streamlines and the average Mg concentration [16].

2.5. Coupled heat flow, fluid flow and solid deformation

As stated before, the thermal field induces stresses and strains in the coherent solid and convection in the liquid region. Fluid flow transports also heat, while deformation of the solid modifies the thermal contact with the bottom block or with the mould. It is therefore necessary to couple these aspects. One of the goals of the POST project [18] is to implement a mixed Lagrangian-Eulerian representation in the 3D code ProCAST [19]. Indeed, a significant difficulty which arises when one wants to model the start-up phase of continuous casting, is the large change in size of the calculation domain in the direction of the casting velocity. This expansion cannot be accounted for by simply deforming the finite elements: such a method would lead to a severe distortion of the elements with a damaging effect on the accuracy of the calculation. A solution to this problem is provided by the use of a dynamic mesh, i.e. a mesh in which new elements are automatically added during the course of a calculation. The strategy is therefore based on the technique of element activation. All the elements exist in the mesh from the beginning of the calculation so that the total number of elements is constant all over the simulation, but the elements can be active (regular) or inactive. Although present in the mesh, inactive elements are skipped during the assembly process and therefore have no influence on the calculation. A zone made of a sufficient number of layers of inactive elements is defined in the initial mesh between the liquid distribution system and the moving part of the casting. When the material begins to move following the bottom block, the nodes in the expanding domain will move at the same speed because of the Lagrangian nature of the description in this region. The layer of inactive elements in contact with the active region is activated and the corresponding elements are stretched to account for the expansion of the domain. As soon as the thickness of this transition layer reaches a given value, the elements get fixed in size and the next layer of inactive elements is activated. The inactive elements act as a reservoir which compensates for the expanding size of the domain by progressive stretching and activation. The behavior of this set of elements mimics the unfolding of an accordion: this is why it is called below the "accordion domain" (see Figure 5). Periodic boundary conditions are used to ensure that the layers of inactive elements have no effect on the calculation, in other words, to ensure the continuity of the solution from one side of the accordion domain to the other side.

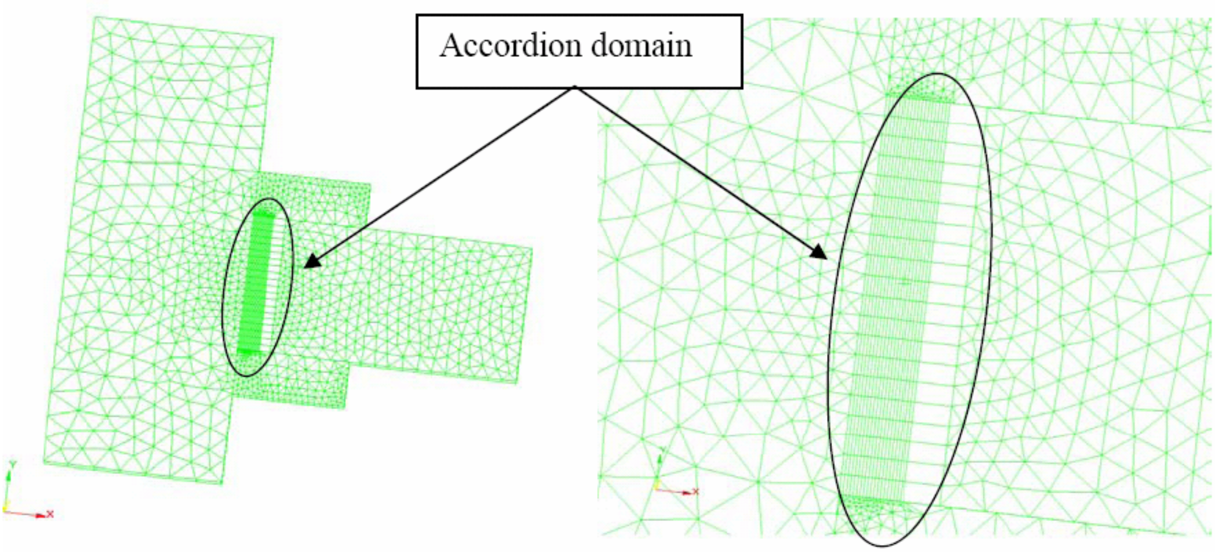

Figure 5: Automatic generation of the accordion domain. The thickness of the elements is set here to a small value to make the elements visible. One layer of elements of the accordion domain is already stretched (POST project, [18]).

3. Microscopic Modelling

3.1. Grain structure formation

In continuous casting, grain structure formation has to consider the nucleation of grains, the fragmentation of dendrite arms and grain growth at a microscopic scale, the motion of the grains and their thermal history at a macroscopic scale. All these phenomena are of course influenced by the temperature field and by fluid flow. Conversely, the presence of equiaxed grains modifies the apparent viscosity of the fluid and their movement also transports heat (and solute). As these phenomena are fairly complex, a semi-coupled approach can be made: the macroscopic aspects of the process are first calculated using appropriate average conservation equations (and thermo-physical data [20]). Then, the motion and growth of equiaxed grains are calculated as a "post-processing" module, using as input the local heat extraction and the velocity field computed at the macroscopic scale.

For Cu based alloys, the influence of electromagnetic stirring (EMS) on grain refinement has been studied in a Bridgman furnace by Campanella and co-workers [21]. Metallographic inspection of the specimens, temperature measurements and numerical simulations performed with CalcoSOFT [22] revealed that the efficiency of EMS is strongly dependent upon the penetration of the liquid in the mushy zone and therefore upon the position of the convection vortices with respect to the liquid front. The results were analysed on the basis of a dendrite fragmentation criterion similar to Fleming's criterion for local remelting of the mushy zone. The new criterion tells that local remelting occurs when the component of the fluid flow velocity along the thermal gradient becomes larger that the speed of the isotherms, as depicted in Figure 6.

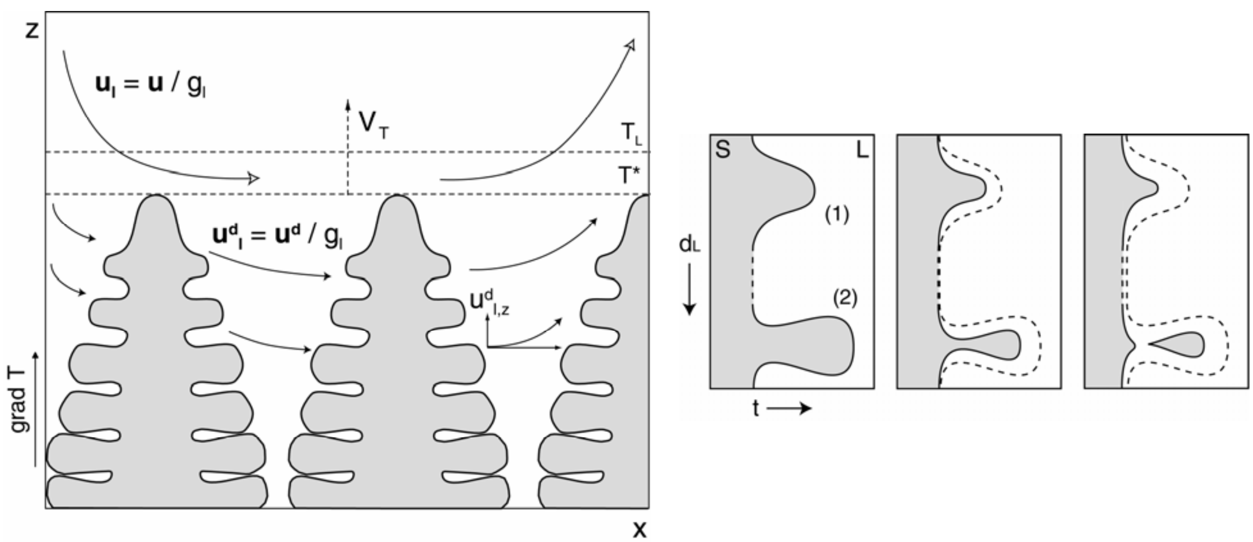

Figure 6: Schematic representation (left) of local fluid flow in the liquid, $\boldsymbol{u_l}$, and in between the dendrites, $\boldsymbol{u^d_l}$. The projection of $\boldsymbol{u^d_l}$ on the thermal gradient (parallel to the z-axis), $u^d_{l,z}$, has to be compared with the velocity of the isotherms V_T . On the right, schematics of remelting (1) and fragmentation (2) of secondary dendrite arms [21].

3.2. Microstructure formation

The prediction of the macro- and microstructures obtained at the end of solidification is of great interest for aluminium producers. Indeed, the mechanical properties of aluminium alloys, but also defects such as hot tearing, are strongly dependent upon these parameters. This is probably why the phase-field method has attracted the attention of so many scientists over the past decade [23-26]. Indeed, with a fixed mesh, such a model is capable in principle to predict the formation of dendrites, eutectics, peritectics, etc ... It can directly use information coming from phase diagram calculations. Nevertheless, it has some inherent difficulties. In particular, the mesh must be fine enough (typically 0.1 micron) to correctly predict the curvature and the diffusion field around a dendrite tip, thus making the time step of the explicit scheme small as well. This makes the calculations CPU intensive and limits the applications to domains of typically 1 mm in size or less, unless adaptive meshes are used.

3.3. Microporosity formation

Although probably less important than hot tearing for DC casting, microporosity is the key defect in shape castings. While resulting from the same combined effects occurring within the mushy zone, namely solidification shrinkage and gas segregation, this defect is usually classified into shrinkage and gas porosity. Taking into account these two phenomena, a quite general module has been developed within the software CalcoSOFT [27]. Darcy's and mass conservation equations are solved only for the mushy zone, using a dynamic and regular finite volume grid superimposed to the fixed finite element mesh used to solve the thermal exchanges within the casting. In this way, an accurate description of the shrinkage-induced pressure drop in the mushy zone can be obtained. Appropriate boundary conditions have to be set at the limit of the mushy zone, taking into account free liquid pockets (regions directly connected to ambient air), closed pockets (regions of liquid totally surrounded by the solid and/or mould) and semi-open regions of liquid (regions of liquid connected to an open region through the mushy zone). At the same time, segregation of gases such as hydrogen is calculated in each volume element. Using the pressure and temperature fields, conditions for the nucleation and growth of pores are then determined, taking into account the important overpressure associated with the curvature contribution. Knowing the amount of microporosity formed in each volume element, macroporosity in hot spots and pipe shrinkage at free surfaces can be deduced simultaneously.

3.4. Hot crack formation

Modelling of hot cracking is probably one of the most challenging issues in solidification. Indeed, it involves thermal stresses/strains of the coherent solid, transmission of these deformations to the partially coherent mush and interdendritic liquid feeding. For many years, very simple criteria, such as the solidification interval, were used to simply address the composition-dependence of the susceptibility of an alloy to hot cracking [28]. In 1999, however, a new approach, based on Niyama's criterion for microporosity formation [3] was derived at EPFL (so-called RDG model after the names of the authors [29]). Assuming that the strain rate component perpendicular to the thermal gradient at the roots of the dendrites is uniformly transmitted to the non-coherent mushy zone, a simple mass balance combined with Darcy's equation allows us to calculate the pressure drop in the interdendritic liquid induced by these deformations and solidification shrinkage. If this pressure falls below a cavitation pressure, a crack is assumed to form. Due to its simplicity, such a physically-sound approach can be easily implemented as a post-processing calculation of a deformation simulation [30]. In order to refine the RDG approach and be more rigorous in the handling of the solid and liquid interactions, the viscoplastic volume change (dilatation/densification) associated with the thermally-induced deformations in the mush, and thus to the thermally-induced "opening-up" of the dendrite network have been recently included in a compressible model of the mushy zone [31-32]. A challenge in the area of hot cracking, and to some extent of porosity formation, is the description of the gradual transformation of a continuous interdendritic liquid film to a continuous and coherent solid. In low concentration alloys, which are the most sensitive to hot cracking, this is achieved by coalescence or bridging of the primary phase [33-35]. Eventually, the numerous parameters entering the compressible model describing the mechanical behaviour of the mushy zone have been determined not only for binary Al-Cu alloys [36] but also for industrial alloys, such as the AA5182 alloy [37].

4. Conclusion

Like DC casting, the development of models is a continuous process. It evolves with the power of computer, with the increased knowledge gained from experimental observations, with the advent of new numerical techniques (phase field, cellular automata, granular methods, etc.) and with the development of new approaches (hot tearing, two phase method, etc …). Nowadays, macroscopic simulation tools are being routinely used by industry, despite their apparent high cost (hardware, software, training of people, maintenance, creation of data bases and expertise for thermo-physical and other properties, validation, …). Yet, there is not a single company which could imagine not using such tools, since this is the only way to get an increased knowledge of the process and therefore to reduce scrap, improve quality and diminish production costs. New sophisticated methods developed recently by academic partners for microstructure and defect formation will also make their way to industry in the future. This is the next logical step to characterize cast ingots from a metallurgical aspect, thus leading the way to properties prediction.

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