



HAL
open science

Prediction of solidification structures in a 9.8 tonne steel ingot

Benjamin Gerin, Hervé Combeau, Miha Založnik, Isabelle Poitroult, Maya Cherif

► To cite this version:

Benjamin Gerin, Hervé Combeau, Miha Založnik, Isabelle Poitroult, Maya Cherif. Prediction of solidification structures in a 9.8 tonne steel ingot. IOP Conference Series: Materials Science and Engineering, 2020, 861, pp.012032. 10.1088/1757-899X/861/1/012032 . hal-02978770

HAL Id: hal-02978770

<https://hal.science/hal-02978770>

Submitted on 23 Dec 2020

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.



Distributed under a Creative Commons Attribution 4.0 International License

PAPER • OPEN ACCESS

Prediction of solidification structures in a 9.8 tonne steel ingot

To cite this article: B Gerin *et al* 2020 *IOP Conf. Ser.: Mater. Sci. Eng.* **861** 012032

View the [article online](#) for updates and enhancements.



The banner features a background image of Earth from space. On the left, there are three circular logos: the top one is 'ECS' in a white circle, the middle one is 'The Electrochemical Society' with a stylized 'ECS' logo, and the bottom one is 'THE KOREAN ELECTROCHEMICAL SOCIETY'. The main text in the center reads 'Joint International Meeting PRiME 2020 October 4-9, 2020' in white and blue. Below this, a blue bar contains the text 'Attendees register at NO COST!' in white. On the right side, there is a large blue logo for 'PRiME' with 'PACIFIC RIM MEETING ON ELECTROCHEMICAL AND SOLID STATE SCIENCE' underneath, and '2020' in large white numbers. At the bottom right, a blue bar contains the text 'REGISTER NOW' with a white arrow pointing right.

Prediction of solidification structures in a 9.8 tonne steel ingot

B Gerin¹, H Combeau¹, M Založnik¹, I Poitraul² and M Cherif²

¹ Université de Lorraine, CNRS, IJL, F-54000 Nancy, France

² ArcelorMittal Industeel, 56 rue Clemenceau, F-71201 Le Creusot, France

E-mail: benjamin.gerin@univ-lorraine.fr

Abstract. The control of the carbon macrosegregation level in steel ingots is important for the structural integrity of the final component. Previous studies using the SOLID® multiscale modelling software have shown that in order to obtain predictive results for the macrosegregation and the grain structure (CET, grain morphology) in steel ingots, a model needs to account for fragmentation of columnar dendrites as a source of equiaxed grains. The goal of this study is to show that a numerical model that takes into account fragmentation can describe the formation of the structures and the macrosegregation during solidification of a large steel ingot. The present article describes how fragmentation is taken into account in the multiphase numerical model used in the simulations. The simulation results are compared to experimental data from a 9.8 tonne ingot cast in A5/6 steel by ArcelorMittal Industeel. The model correctly reproduces the major features of the experimentally observed structure and macrosegregation. We show that the structures are formed very early on during solidification, whereas macrosegregation develops much more gradually. Our results also underline the importance of liquid flow and grain movement in order to correctly predict the final structure and macrosegregation.

1. Introduction

Achieving homogeneous mechanical properties for large cast ingots is an industrial challenge because of the segregation of alloying elements during solidification. This is due to an enrichment of the liquid in alloying elements as solidification progresses. This can lead to large-scale inhomogeneity (macrosegregation) which will affect the local mechanical properties. Being able to predict and control macrosegregation is thus crucial for the structural integrity of the components.

Segregation is the result of the complex interaction of the solidification structures (columnar, equiaxed, grain morphology) and liquid flow. Additionally, the structures themselves can influence mechanical properties, so accurately predicting both the macrosegregation and the solidification structures is an important issue for steel ingot producers. The prediction of the structures requires taking into account the fragmentation of the columnar dendrites in the model [1]. The present study uses the SOLID® multiscale and multiphysics model to predict the structure and macrosegregation of a 1.44 m diameter, 9.8 tonne steel ingot by taking into account the fragmentation during solidification. The originality of this study lies in the prediction and description of the formation of the structures and the macrosegregation, which is not commonly found in literature for such large products.

Fragmentation of the columnar dendrites happens when secondary dendrite arms detach and are swept in the bulk liquid. If the local conditions are favourable, they will grow as equiaxed grains before sedimenting at the bottom of the ingot, leading to a columnar to equiaxed transition. Fragmentation is an important source of equiaxed grains, especially in castings with no inoculation. The detachment of secondary arms does not occur because of mechanical breakage [2] but rather due to local dissolution at



the root of the secondary arms [3] or remelting of the arms due to temperature increase [4]. During normal coarsening of the columnar structure, secondary arm detachment is quite slow. However, certain situations massively increase fragmentation, such as unconstrained growth of the columnar front [5] or slowdown of the columnar tip velocity [6]. In addition, in steels, the peritectic transformation can also promote the increase in size of the equiaxed region [7].

2. Model used in the SOLID[®] software

The SOLID[®] software, developed on scientific models from IJL, supported by a French consortium of industrials in the framework of metallurgy and supported also by national and European funding is commercialized by SCC (see www.sconsultants.com) to be released in the industry. SOLID[®] uses a 2D finite volume method to discretise the set of partial differential equations of a multiphase model (liquid, columnar, equiaxed and inter-dendritic liquid for both solid phases). Each discretised volumetric element, or "cell" can contain both columnar and equiaxed solid, in addition to liquid. Cells containing both columnar and equiaxed grains are called mixed cells. Solidification begins with a columnar front starting on the mould walls which can grow and fragment. Fragmentation generates equiaxed grains in the undercooled region ahead of the columnar front. These equiaxed grains are not individually simulated but are instead represented by average grain size and grain density values in each cell. Fragmentation is implemented using the model developed by Nicolas Leriche in his PhD [8]. Fragmentation uses two parameters: the fragmentation flux density (number of generated grains per surface area of columnar front per second) and the thermal gradient activation threshold. The threshold means that the fragmentation occurs only when the temperature gradient at the columnar front is locally smaller than a given threshold value.

The model calculates the movement of the liquid phases (bulk liquid and inter-dendritic liquid inside the grain envelope) and of the equiaxed grains. There is a complex interaction between liquid flow and grain movement, each influencing the other. The grains can be swept up by the liquid flow and grow or remelt depending on local undercooling. Generally, small grains (< 1 mm) will follow the liquid movement, whereas larger grains have enough mass that the liquid flow cannot overcome their downward movement, and they sediment at the bottom of the bulk liquid. Grain movement in a cell is blocked when the liquid fraction is below 0.6. Additionally, there is no grain movement in cells containing columnar grains. The columnar front in a cell is blocked when the envelope fraction of equiaxed grains in that cell reaches 0.5, leading to a columnar to equiaxed transition (CET). Unlike the columnar structure, equiaxed cells cannot progress from one cell to the next. However, they can generate an equiaxed to columnar transition (ECT), producing new columnar cells. In the model, ECT is set to occur only if there are no equiaxed grains in the surrounding liquid. When ECT starts, a new columnar front is started in the adjacent liquid cells, which can then grow, fragment and can itself be blocked. Further information about the model can be found in previously published work [9].

3. Structures and macrosegregation experimentally observed in the 9.8 t ingot

The focus of the present article is a 9.8 t experimental research ingot cast in A5/6 steel by Industeel. It has a diameter of 1.44 m and a height of 0.74 m, which is much smaller than typical commercial Industeel ingots. This ingot was cast specifically for research purposes and was not destined to produce a component. Ingots of this shape (large diameter compared to height) are used to make flat component such as thick plates and disks [10]. The composition of the alloy, measured just before casting, is given in table 1.

Table 1. Chemical composition in wt% of the A5/6 steel used in the 9.8 t ingot.

C	S	P	Si	Mn	Ni	Cr	Mo	Cu	Sn	Al	Fe
0.184	0.026	0.008	0.245	0.59	0.17	0.23	0.035	0.250	0.025	0.018	Balance

The mould is made of cast iron and there is no hot top, however the liquid metal is covered by two layers of powder: an exothermal powder with an insulating powder on top. The total solidification time was less than 6 hours. After solidification, the ingot was cut in half along a diameter in order to analyse its macrostructure and segregation. Figure 1 shows the schematic representation of macrostructures such as dendrites and equiaxed grains, identified with a macro-etching. The different macrostructures were visually identified and manually colour-coded.

The stand-out features have been numbered in figure 1: the primary columnar region along the side and bottom walls (1); an equiaxed structure with fine grains (2) on the bottom and larger grains on top (3); a thin layer of equiaxed grains (4) separating the primary columnar with the central columnar region (5). Above the equiaxed region, a large ‘step’ in columnar thickness is visible (6). The top of the ingot is mostly columnar, with the centre region being a mix of columnar and equiaxed grains.

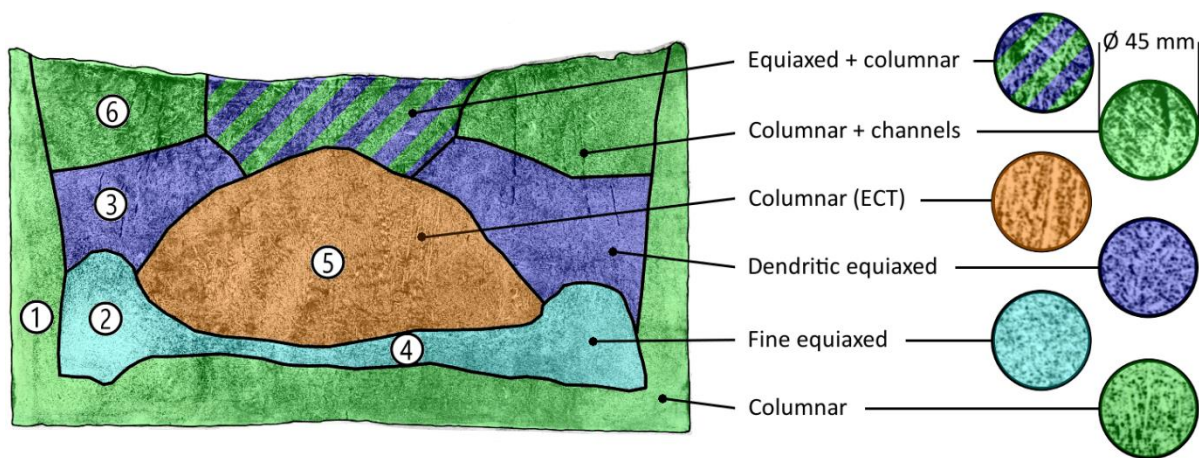


Figure 1. Experimentally observed structures of the 9.8 t ingot.

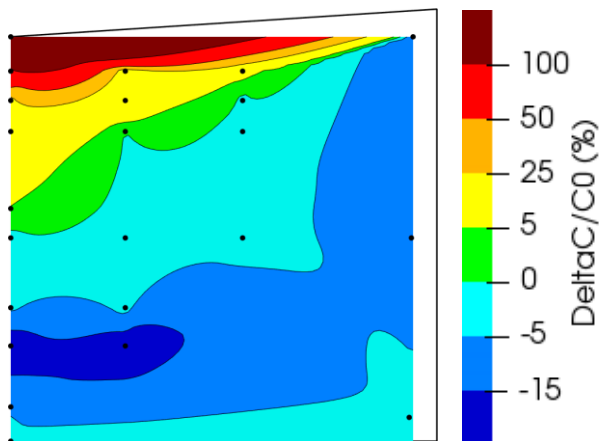


Figure 2. Experimental measurements of carbon concentration in a cross-section of the ingot, represented as percentage variation of nominal composition $\Delta C/C_0$. Contour lines were obtained by interpolating the experimental data. Only half of the ingot is represented, the centreline is on the left. Minimum value is -23% and maximum value is $+290\%$.

Analysis was performed on the open face of the ingot cross-section to measure carbon segregation. The experimental measurements of carbon concentration are presented in figure 2. Each data point is located by a black dot and its value is given as a percentage variation of the nominal concentration $\Delta C/C_0$. The experimental data was interpolated in order to plot contour lines. The bottom part of the ingot is negatively segregated, reaching -23% of the nominal composition. The top centre region, which is the last to solidify, features a large positive segregation, with a maximum of $+290\%$ relative to the nominal composition.

4. Numerical simulation

The solidification of the 9.8 t ingot was simulated using the SOLID[®] software using an axial symmetry. In order to simplify the calculation, a binary Fe–C alloy is used, with 0.184 wt% carbon. The fragmentation parameters were determined by performing a sensitivity analysis on these parameters (not discussed in this article), and then choosing the values that gave the results closest to the experimental ingot. The chosen fragmentation parameters are: fragmentation flux density of 500 frag.m⁻².s⁻¹ and activation of fragmentation at a thermal gradient below 26 K.m⁻¹. Both exothermal and insulating powders are present in the simulation. The exothermal reaction is simulated using an enthalpy of reaction, leading to an increase in temperature of the powder. The chosen enthalpy of reaction in this simulation leads to a powder temperature significantly lower than the liquidus of the alloy ($T_{exo} < T_{liquidus}$). Additionally, the formation of columnar grains is disabled on the top surface of the ingot, where the liquid metal is in contact with the exothermal powder. Filling is taken into account using a simplified line by line filling method. The simulation uses a mesh size of 1 cm, so the total number of cells is 21643 of which 5697 are for the ingot. With a time step of 0.1 s, the total computation time on one CPU core was 40 hours. Coarser mesh sizes give similar results, with a roughly equivalent columnar thickness.

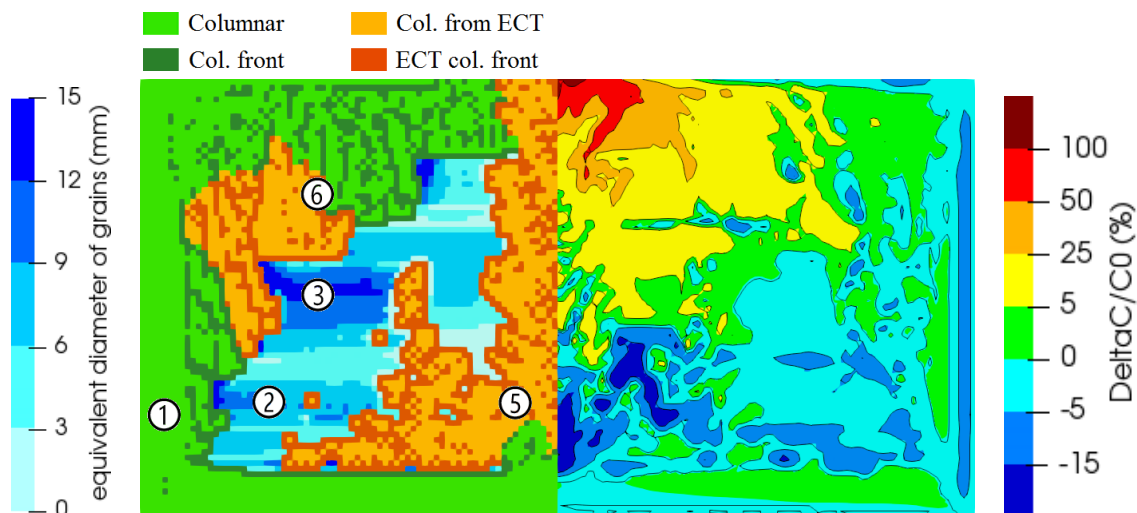


Figure 3. Simulation results for the 9.8 t ingot. The structure map is given on the left side, showing the columnar structure (either primary or from ECT) and the grain diameter for the equiaxed structure. On the right side, the carbon composition is given as a percentage of nominal composition.

The final structure map and carbon segregation pattern at the end of the simulation are given in figure 3. The same structure colour code was used as in figure 1: green and orange for columnar, blue for equiaxed. In addition, mixed columnar-equiaxed cells are distinguished by a darker columnar colour (dark green or dark orange).

The simulated macrosegregation is similar to the experimental results (figure 2), with a negative segregation reaching -34% in the bottom part of the ingot and a large positive segregation in the top part, with the maximum value ($+129\%$) along the centre axis. The transition from negative to positive segregation along the axis happens at a similar point, roughly half the height of the ingot. The simulated structures also show similarities to the macrographic etching (figure 1), with almost all major features being reproduced. These have been numbered the same way as in figure 1: the primary columnar on the mould wall (1); the equiaxed region (2) of small grains (mostly smaller than 9 mm) with the transition to larger grains (3) (greater than 9 mm); the large central ECT region (5); and the ‘step’ in columnar thickness (6) above the equiaxed region. However, the layer of equiaxed grains separating the primary columnar from the center columnar (4) in figure 1, is missing. Additionally, the thickness of the primary columnar is overall greater in the simulation than in the experimental data.

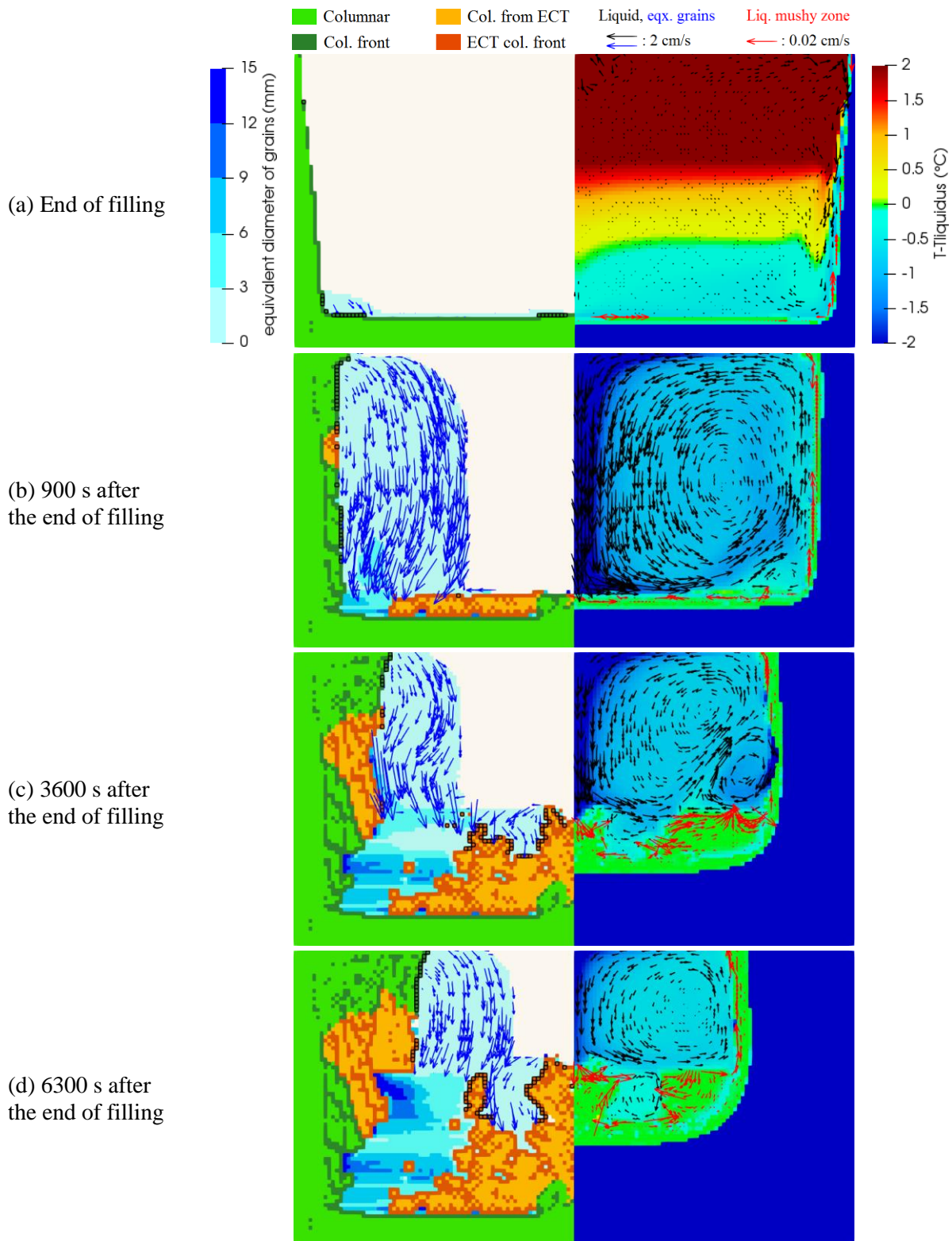


Figure 4. Simulation results for the 9.8 t ingot. The left side shows the columnar structure, with fragmenting cells outlined in black, the equiaxed grain diameter and grain movement (blue arrows). The right side shows $T - T_{liquidus}$ (positive: superheated; negative: undercooled), the liquid movement in black arrows, and the liquid movement in the mushy zone is in red arrows.

5. Discussion

The simulation shows the entire solidification sequence, explaining when and how the various structures were formed. The solidification sequence can be divided into the following stages, illustrated in figure 4:

- Solidification starts immediately with a columnar front initiating on the mould walls. Halfway during filling, a few cells start fragmenting at the bottom on the ingot, generating fragments in the liquid ahead of the columnar front.
- At the end of filling (figure 4(a)), the columnar front is already well developed, and the equiaxed grains produced by fragmentation have already blocked the columnar front on the bottom surface. The equiaxed structure starts forming at the bottom from the accumulation of sedimented grains. Because of the simplified filling model, there is little liquid convection during filling, and most of the liquid remains in superheat. After filling, convection is much more pronounced due to the heat exchange between the liquid and the exothermal powder (which is colder than the liquidus temperature of the alloy). The liquid loses its superheat 200 s after filling.
- 900 s after filling (figure 4(b)), liquid convection has stabilised into a large vortex with the liquid flowing downward in the middle of the ingot and upward along the columnar front. This movement is due to the liquid being simultaneously cooled at the top by the exothermal powder and enriched in carbon along the columnar front. Because the entire bulk liquid is undercooled, the equiaxed grains grow and sediment quickly. The liquid vortex prevents the sedimenting equiaxed grains (blue arrows) from reaching the centre of the ingot. The grains thus sediment near the mould wall, creating an equiaxed region on the outer edge of the ingot, and allowing the centre columnar region to grow unimpeded. The equiaxed and columnar regions grow upward roughly in parallel, creating the central structure seen in figure 1.
- Around 3600 s after filling, the small corner vortex in the liquid convection becomes much larger, as seen in figure 4(c). For the next 1000 s, the liquid convection has two counter-rotating vortices, after which the smaller corner vortex subsides. This smaller vortex changes the liquid flow along the vertical columnar front: instead of warm enriched liquid flowing upward, cooler less rich liquid is flowing downward. The falling equiaxed grains therefore grow much faster before sedimenting, and the sedimentation of larger grains leads to a rapid progression of the equiaxed region. This region of large equiaxed grains can be seen in figures 1 and 3.
- After the corner vortex disappears (around 4600 s after filling), the sedimenting grains are much smaller in size. This is because the liquid flowing up against the columnar front is enriched and less undercooled, but also because the grains have a shorter distance to grow before blocking. The sedimentation of smaller grains greatly slows down the upward progress of the equiaxed region. This gives time for the columnar front on the mould wall to grow horizontally. This is shown in figure 4(d): at 6300 s after filling, the columnar region on the side has grown horizontally to cover the region of large equiaxed grains. At that time, the ingot is 78% solidified, with the upper part still fully liquid and a small mushy zone in the equiaxed region (the red arrows in the figure shows the liquid convection in the mushy zone). At this stage, most of the macrostructures are already in place but the macrosegregation is still low: the carbon content in the bulk liquid is +15% relative to nominal composition.
- For the remainder of solidification ($t > 6300$ s), there are no major changes to the structure or liquid flow. Total solidification time is around 21300 s, with final solidification in the upper region at the centre of the ingot. The two columnar fronts slowly grow, competing with the equiaxed region to fill the remaining liquid volume. This results in the columnar and equiaxed structures that are visible in the top part of the ingot in figure 3. This final stage of the solidification is by far the longest (15000 s, 70% of total solidification time), during which the macrosegregation continues to evolve slowly due to liquid flow and grain sedimentation.

The simulation has a complex liquid flow that has a large influence on the sedimenting grains, and this ultimately affects the final structure and macrosegregation of the ingot. Liquid flow is driven by thermal convection but also by solutal convection (carbon enrichment reduces liquid density). In the simulation, thermal convection is largely influenced by the temperature of the exothermal powder that

covers the top of the ingot. If the powder is sufficiently colder than the liquidus temperature of the alloy, cooling the liquid, then the liquid will flow downward along the central axis of the ingot. This is the case for the simulation presented in figure 3 and 4, with the resulting convection loop shown in figure 4. The convection generates an outward liquid flow along the bottom part of the ingot, chasing away the sedimenting grains and allowing for the large columnar region in the centre of the ingot. The convection also brings in fresh liquid into the growing columnar front, pushing enriched liquid outward and upward. This creates the region of negative segregation seen at the bottom of the ingot in figure 3. In the current model, this is achieved by using enthalpy of reaction values that give exothermal powder temperatures that are unrealistically low compared to the industrial process. Further work must be done to better understand the influence of the exothermal powder on liquid flow.

Conversely, if the powder is hotter than the liquid, then the top part of the bulk liquid stays hot and the cooling of the liquid happens from the side wall. This creates a convection loop in the opposite direction: liquid is flowing downward along the mould wall and upward along the centre axis. A convection loop in the opposite direction will bring in sedimenting grains and enriched liquid, instead of pushing them away. This drastically changes the macrosegregation and structure in the bottom part of the ingot. Figure 5(a). shows the result of a simulation with $T_{exo} > T_{liquidus}$ (other parameters being identical). The opposite convection loop in this simulation removes the central columnar region and leads to a much less pronounced negative segregation.

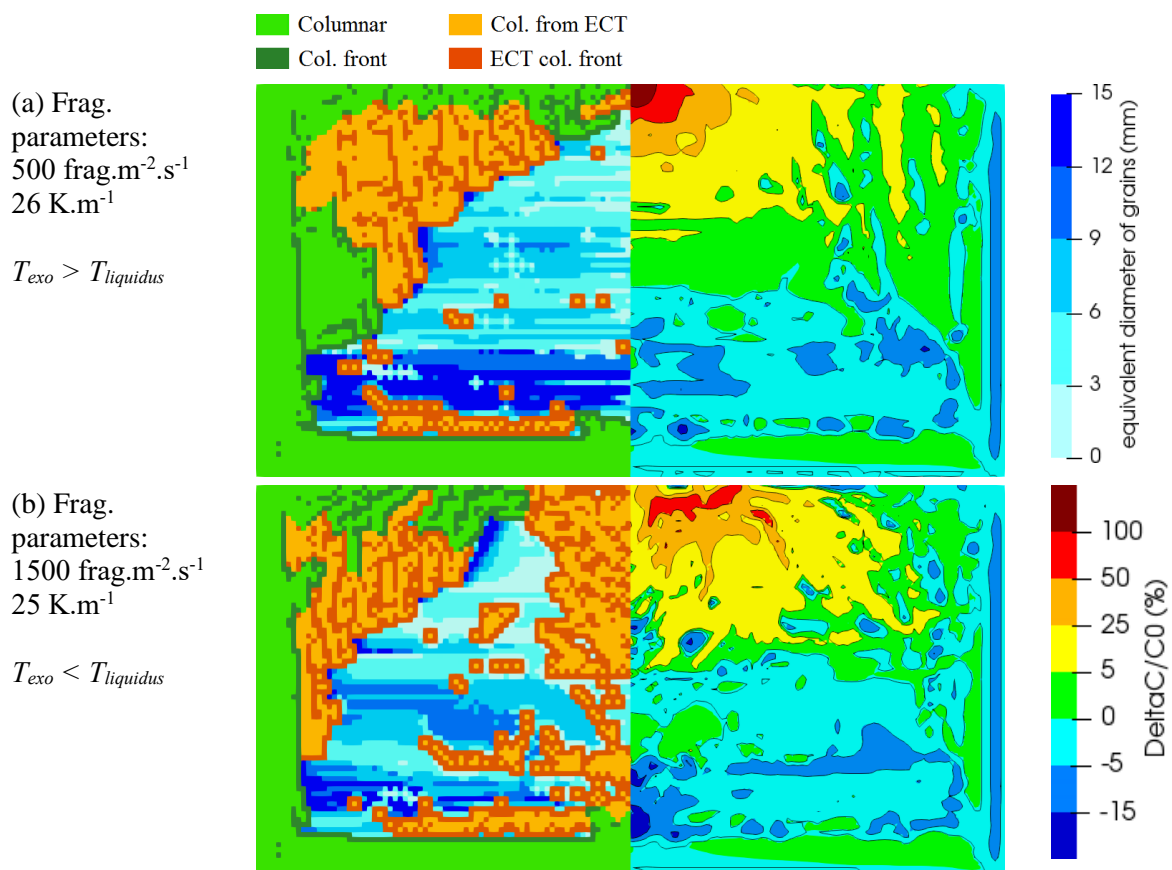


Figure 5. Simulation results for the 9.8 t ingot with different fragmentation parameters and exothermal powder temperatures.

These results show the large influence that liquid movement in the bottom part of the ingot has on structure and macrosegregation. An outward movement along the bottom will lead to a columnar region in the centre, with a pronounced negative segregation. Inward convection will instead lead to an

equiaxed region and a reduced negative segregation. This effect is further illustrated in figure 5(b). In this simulation, the direction of liquid flow changes several times during solidification, and this creates alternating layers of equiaxed and columnar grains in the lower part of the ingot. Furthermore, these columnar regions have corresponding areas of negative segregation.

The absence of convection during filling in the simulations is probably the reason why the layer of equiaxed grains between the primary columnar and the central columnar is missing at the bottom of the ingot. The ingot being bottom poured, this will naturally lead to a large vortex with inward flow along the bottom, thus creating the missing equiaxed layer.

6. Conclusion

The simulation results show that by using only fragmentation as a source of equiaxed grains, it is possible to predict both the macrosegregation of carbon and the complex macrostructure of a steel ingot. The simulations show that liquid flow has a large influence on the development of the structures and the segregation. In addition, most of the structures are formed early on during solidification, 6300 s in our case, 30% of the total 21300 s. Conversely, the large positive segregation forms slowly over a much longer period

However, as the exothermal powder temperature used in the simulations is lower than what is used industrially, further work must be done to understand its effect and improve how it is modelled. Additionally, the lack of convection during filling is another area where the model will be improved.

Acknowledgements

The authors would like to thank the partners of this study for their support: Industeel, EDF, Framatome and Sciences Computers Consultants.

References

- [1] Leriche N, Combeau H, Gandin Ch-A and Založnik M 2015 Modelling of columnar-to-equiaxed and equiaxed-to-columnar transitions in ingots using a multiphase model *IOP Conf. Series: Mat. Sci. & Eng.* **84** 012087
- [2] Pilling J and Hellawell A 1996 Mechanical deformation of dendrites by fluid flow. *Met. & Mat. Trans. A* **27** 229-32
- [3] Neumann-Heyme H, Shevchenko N, Lei Z, Eckert K, Keplinger O, Grenzer J, Beckermann C, and Eckert S 2018 Coarsening evolution of dendritic sidearms: from synchrotron experiments to quantitative modeling. *Acta Mat.* **146** 176-86
- [4] Sato T, Kurz W, and Ikawa K 1987 Experiments on dendrite branch detachment in the succinonitrile-camphor alloy. *Trans. of the Japan Institute of Metals* **28(12)** 1012-21
- [5] Gandin Ch-A 2000 From constrained to unconstrained growth during directional solidification. *Acta Mat.* **48(10)** 2483-501
- [6] Liu S, Lu S-Z and Hellawell A 2002 Dendritic array growth in the systems NH₄Cl-H₂O and [CH₂ CN]₂-H₂O: the detachment of dendrite side arms induced by deceleration. *J. of Crystal Growth* **234(4)** 740-50
- [7] Tiwari S N and Beech J 1981 The role of the peritectic reaction in the formation of the equiaxed zone in iron base alloys. *Trans. ISIJ* **21** 554-8
- [8] Leriche N 2015 *Etude de la Transition Colonnaire-Equiaxe dans les Lingots et en Coulée Continue d'Acier et Influence du Mouvement des Grains*. Phd Thesis, Université de Lorraine, Nancy
- [9] Combeau H, Založnik M, Hans S, and Richey P E 2009 Prediction of macrosegregation in steel ingots: influence of the motion and the morphology of equiaxed grains. *Met. & Mat. Trans B* **40** 289-304
- [10] Benhamou C, Poitault I, Pisseloup J and Bocquet P 1985 Application of directional solidification ingot (LSD) in forging of PWR reactor vessel heads. *10th Int. Forging Conf.* 23-5