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Continuous Casting of High Carbon Steel: How Does Hard Cooling Influence Solidification, Micro- and Macro Segregation?

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Abstract. One technology that is often employed in continuous casting of high-carbon steel billets to minimize centre- (or macro) segregation is hard secondary cooling. Investigations unanimously show, that hard cooling significantly reduces macro-segregation, but a mechanism for the reduced segregation is rarely given. In this paper the solidification of high carbon tire cord grade C80D cast as a 150x150 mm billet is calculated using the proprietary SMS Group solidification simulation package CHILL using steel properties calculated with the Thermo-Calc Software package and TCFE steels database. The obtained cooling rates in the billet for hard and soft secondary cooling are used to run solidification simulations considering solute redistribution using the diffusion module DICTRA. It is shown that for cooling rates achieved in continuous casting the steel solidifies far away from equilibrium. The solidification profile and solidus temperature lie in between the Scheil solidification model and the para-equilibrium Scheil model with carbon defined as a fast diffusing element. The calculated cooling rates and temperature gradients are used to simulate the solidification microstructure 20 mm from the billet surface using the phase field approach and the MICRESS® software package linked to Thermo-Calc through the TQ interface. This model clearly shows, that the most probable mechanism by which hard cooling reduces segregation is trapping of solutes between the intricately branched dendrite microstructure that results from the steep temperature gradients achieved when applying hard secondary cooling.

1. Introduction

The chemistry of tire cord steel is simple, the main alloying element being carbon only. It is however challenging to produce as macro- or centre segregation during continuous casting must be minimized and very stringent requirements on steel cleanness must be met. These factors are important, because the steel is drawn to very thin gauges of 0.15 mm and even below. A single 150x150 mm square billet thus yields ~15'000 km of wire and the thinner the gauge the higher the likelihood becomes of wire breakages, initiated either by non-deformable inclusions or by martensite spots that result from high centre segregation.

A technology to reduce segregation in continuous casting of billets is "hard-cooling" ([1] and references therein). In this process the billet surface is cooled to 300-500°C in the spray chamber with high intensity water spray cooling. The mechanism by which this reduces segregation has still not been fully clarified. This paper by no means has the ambition to present a detailed and exhaustive investigation, it merely aims to introduce various fundamental concepts that are at play during the solidification of continuously cast billets at different cooling rates. Simulations are performed use thing the Thermo-Calc Software package [2], Thermo-Calc's diffusion module DICTRA [3][4], the phase-field based microstructure evolution simulation package MICRESS® [5] and the SMS Goup's proprietary solidification simulation program for continuous casting CHILL [6]. For all

calculations the high carbon steel grade C80D (EN 1.0622, SAE 1080, DIN C80D) is used with a highly simplified composition of 0.8 wt% C and 0.6 wt% Mn so that all equilibrium and diffusion calculations can be reproduced by the interested reader using the freely available Thermo-Calc DEMO version and the free databases FEDEMO and MFEDEMO that can be downloaded from the Thermo-Calc web page [7]. For calculations with more realistic alloy compositions including other elements the commercial TCFE9 and MOBFE4 are required.

2. Equilibrium Solidification of C80D

Phase diagrams are the basis for understanding any metallurgical process. *Figure 1* shows the calculated Fe-C isopleth with constant Mn content of 0.6 wt% (left) and the corresponding equilibrium phase fractions for C80D with 0.8 wt% C and 0.6 wt% Mn (right).
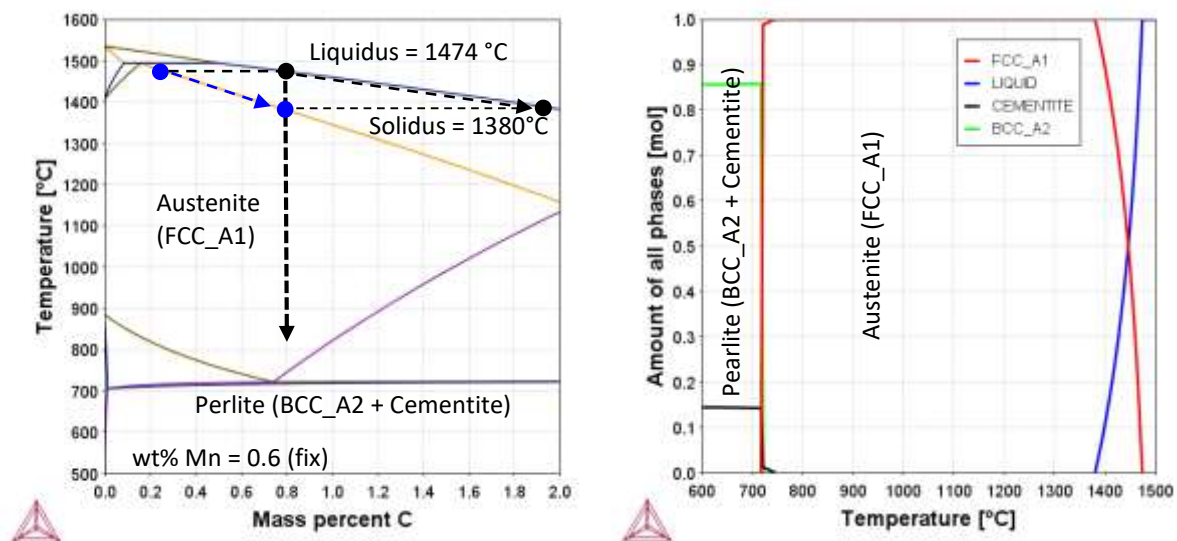

Figure 1. Isopleth of the Fe-C-Mn system at 0.6 wt% Mn (left) and equilibrium phase fractions in function of temperature of the composition Fe - 0.8 wt% C - 0.6 wt% Mn.

Under equilibrium conditions (full solute redistribution, infinitely slow cooling rate) pure Austenite (FCC_A1) forms on solidification with a liquidus- and solidus temperature of ~1474°C and 1380°C respectively. The Austenite decomposes into BCC and Cementite (Perlite) close to the eutectoid composition at ~720°C. The points and arrows in the phase diagram indicate the change in composition required in the solid and liquid phase under equilibrium conditions. In reality, the steel chemistry of grade C80D will be much more complex with tramp and trace elements resulting in slightly different solidus and liquidus temperatures and many other phases including oxides, carbides, nitrides or sulphides might precipitate. All these reactions can be accurately calculated using Thermo-Calc and the commercial TCFE9 database.

3. Scheil-Gulliver Solidification Model and Solidification Considering Back Diffusion

Real solidification processes are too fast for complete homogenization of the solid phase to occur. This means, the equilibrium solidification path (lever-rule) as shown in *Figure 1* is not applicable. An alternative solidification calculation is the Scheil-Gulliver (or simply Scheil) model [8]. It considers local equilibrium at the solid-liquid interface but assumes that no diffusion takes place in the solid phases. These thus become progressively richer in the solute elements from centre to shell, like an onion, as solidification progresses (*Figure 2*). In the liquid uniform solute distribution is assumed. The liquid becomes richer and richer in the solute as solidification progresses resulting in a marked depression of the solidus temperature.

Carbon dissolves interstitially in steels and diffuses very quickly. So Scheil's assumption of no diffusion in the solid is invalid. The assumption of equilibrium solidification is also invalid as the substitutional elements (Mn in our case) diffuse very slowly. This dilemma can be resolved by applying a partial equilibrium- or para equilibrium Scheil model, where one or more elements are defined as "fast diffusing". This is done by setting the chemical potential of the fast diffusing element(s) in the whole phase equal to their chemical potential at the phase boundary. Mathematically this corresponds to infinitely fast diffusion of these elements. In *Figure 3*

Scheil solidification of the simplified C80D steel is compared assuming no diffusion of carbon (left) and fast diffusion of carbon (right).
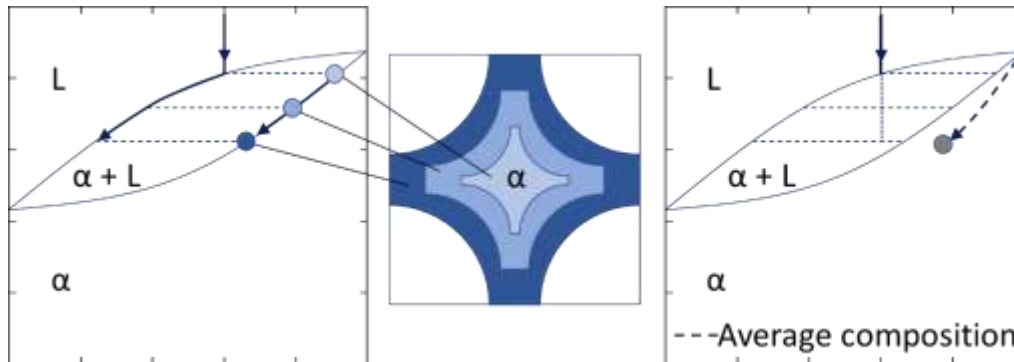

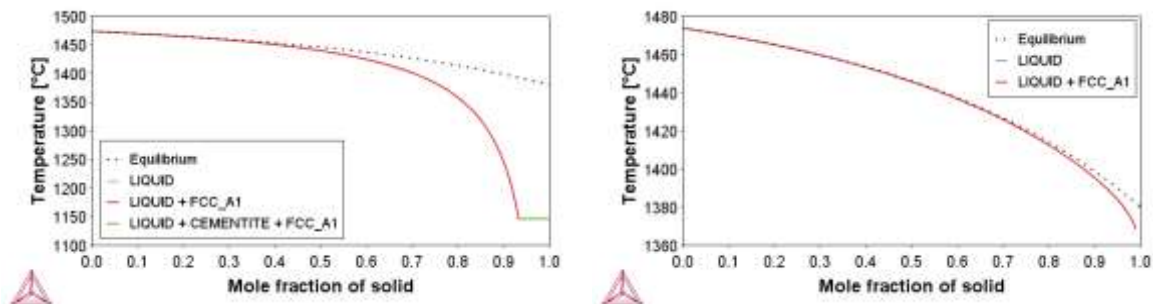**Figure 2**. Visualisation of the Scheil solidification model.

Figure 3. Scheil solidification simulation assuming no diffusion in the solid phase (left) showing large depression of the solidus temperature and precipitation of primary cementite (left) compared to Scheil solidification simulation with C defined as fast diffusing element. Please note the different temperature scales!

   The former predicts a solidus temperature of ~1150°C and the precipitation of primary cementite. In normal casting conditions this is not observed. Setting C as a fast diffusing element results in a more realistic depression of the solidus temperature by about 20°C to 1360°C compared to equilibrium solidification. Which of the solidification models outlined above is more appropriate depends on the cooling rate. Equilibrium solidification corresponds to infinitively slow cooling, Scheil solidification without fast diffusion of C corresponds to such a fast cooling rate that even C does not have enough time to diffuse. Scheil solidification with fast C diffusion corresponds to some intermediate cooling rates that allows enough time for C to diffuse, but not enough time for all other element (in our case Mn) to diffuse. If we want to understand which model is most appropriate, we must first know the cooling rates obtained in continuous casting. Then quantitative diffusion calculations using Thermo-Calc's diffusion module DICTRA can be performed.

4. Solidification simulation of continuously cast 150x150 mm billet

The state-of-the-art solidification simulation model CHILL developed by the SMS Group for the on-line and real-time simulation of the continuous casting process of long products was used to calculate the solidification of a 150x150 mm square billet. Casting speed is 2.2 m/min and the specific secondary cooling volume is 0.8 l/kg for soft cooling and 2.2 l/kg for hard cooling. A standard 9 m billet caster design is used with 1 m CONVEX® copper mould tube and standard water-only secondary spray cooling design. The steel properties used for the simulation (enthalpy, thermal conductivity and volume) are all calculated by equilibrium calculations using Thermo-Calc and the TCFE9 steels database.

   Figure 4 shows the calculated billet solidification profiles (fraction solid 0 and fraction solid 1 isotherms in the billet, top inserts) and the surface temperature and the temperature 20 mm below the billet surface for the two secondary cooling intensities.
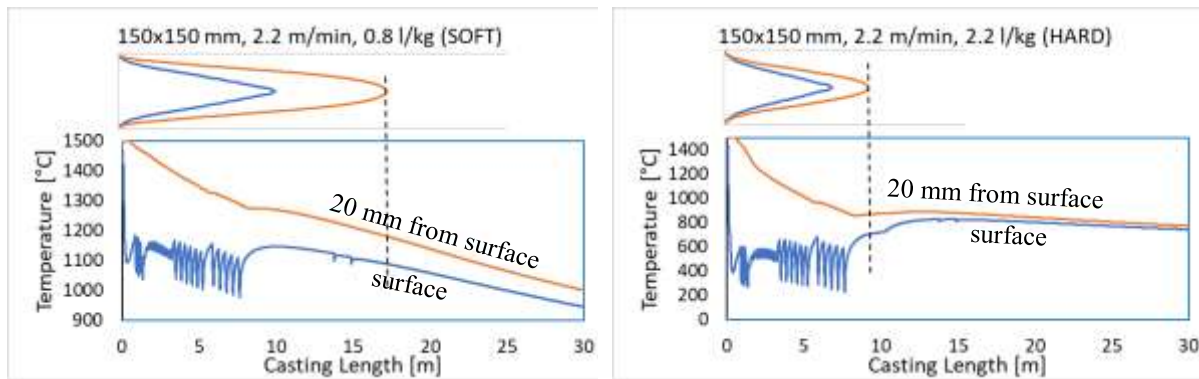
Figure 4. Solidification profiles for 150x150 billet. The calculated solidus and liquidus profiles in the billet are shown at top, at the bottom the surface temperature (blue) and the temperature 20 mm from the billet surface is shown. Please note the different scale!

5. Solidification Simulation Considering Full Diffusion

The time-temperature relation 20 mm from the surface of the 150x150 mm billet as calculated in the preceding section is used for the following solidification calculated under full quantitative consideration of the back diffusion in both the liquid and solid phase. The calculation domain is a small pool of liquid with a width of 0.5 mm that is trapped between secondary dendrite arms 20 mm below the billet surface. The diffusion equation is solved using the diffusion module DICTRA with the free mobility database MFEDEMO. The driving force for diffusion (gradients in chemical potentials) are calculated using Thermo-Calc and the free database FEDEMO. *Figure 5* (left) shows how the solid-liquid interface moves for the two cooling rates. This could be interpreted as the thickening of the dendrites in function of time and temperature. In the case of hard cooling, solidification of the small 0.5 mm volume is completed in ~40 sec. For soft cooling solidification takes ~160 sec. Note that the movement of the solid-liquid interface has nothing to do with the "shell growth" of the billet, rather it corresponds to the rate at which tiny pools of liquid that are trapped between the secondary dendrite arms solidify and disappear. Or in other words, it corresponds to the time required for our small volume of liquid to cool from the liquidus temperature down to the solidus temperature.
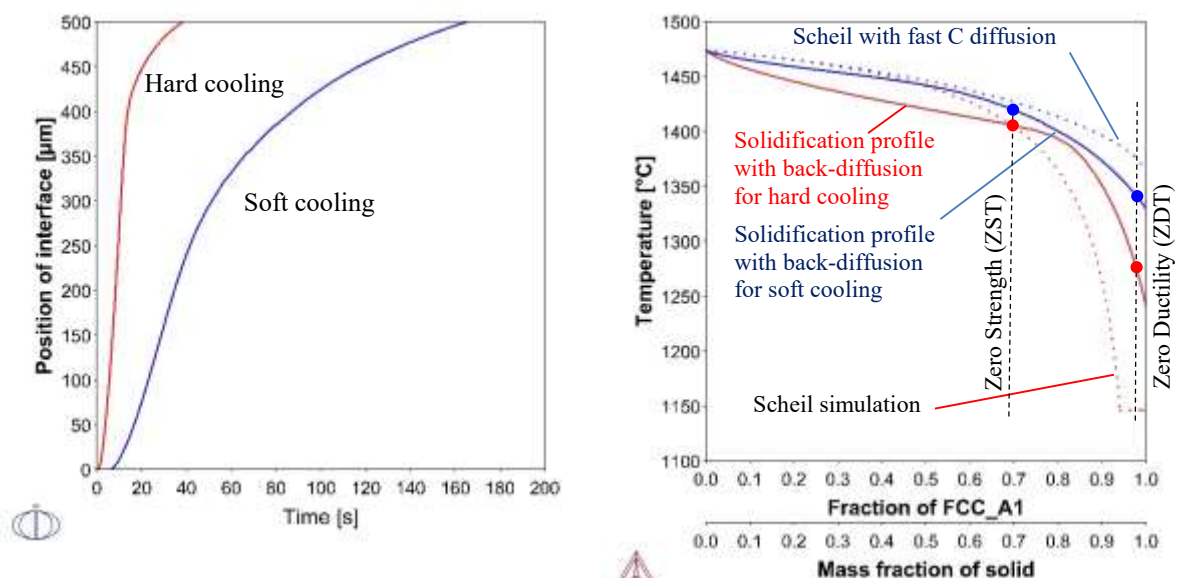

Figure 5. Position of solid-liquid interface in function of time for hard and soft cooling (left) and fraction solid curves (right) considering back-diffusion compared to the results from the Scheil calculations

As the solidification front moves it pushes highly segregated liquid ahead of itself that depresses the solidus temperature as shown in *Figure 5* (right). This thin but pronounced layer of C and Mn rich liquid is more

pronounced for hard cooling as the interface moves faster (**_Figure 6_**) leaving less time for the back-diffusion of the elements. This layer is also the source of interface instability that results in the formation of dendrites due to constitutional undercooling.
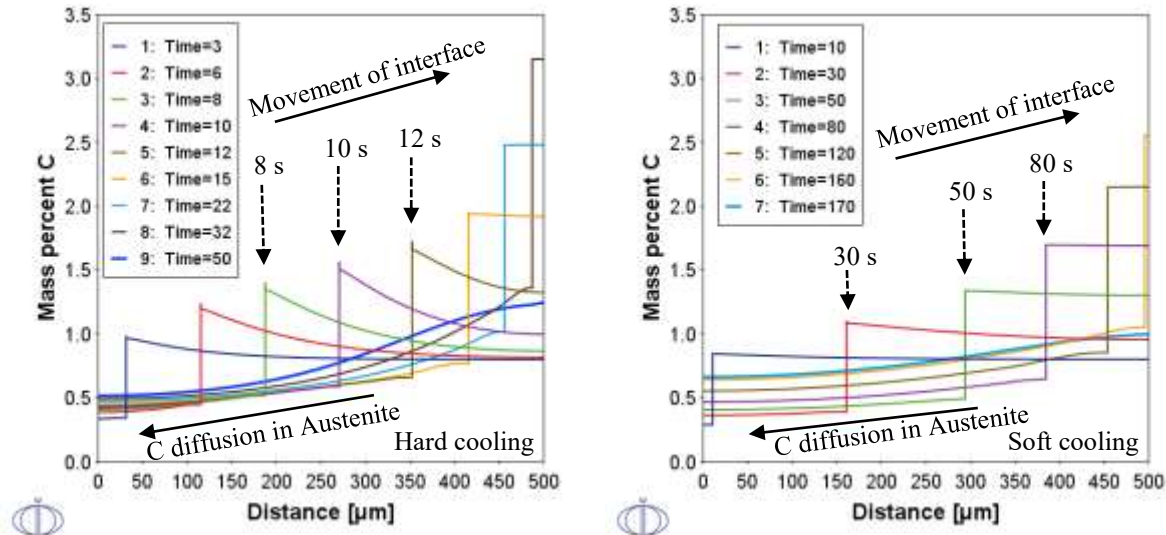

Figure 6. Carbon concentration in function of position and time. For hard cooling the pronounced concentration peak ahead of the solidification front can be clearly seen.

Internal cracks or hot tears (**_Figure 7_**) are a serious problem in continuous casting. The susceptibility to crack formation is closely related to the solidification process. When the solid fraction is low the steel behaves like a liquid. The steel flows and consequently has no mechanical strength and cracks cannot form. As the solid fraction gets higher, the space between dendrites decreases until at a certain temperature bridges start forming between the dendrites. This temperature is known as the "Zero Strength Temperature" (ZST) and is usually assumed to correspond to a fraction solid of ~0.6 – 0.8. Below this temperature brittle fracturing of the steel can occur: the weak bridges between dendrites are broken and the crack is usually filled by highly segregated liquid from between the dendrite arms. On lowering the temperature further, the amount of inter-dendritic liquid is reduced and the bridges between the dendrites become stronger until at one point the ductility is no longer zero. This temperature is referred to as the "Zero Ductility Temperature" (ZDT) and is generally assumed to correspond to a fraction solid of 0.99 or 1 [9] [10].
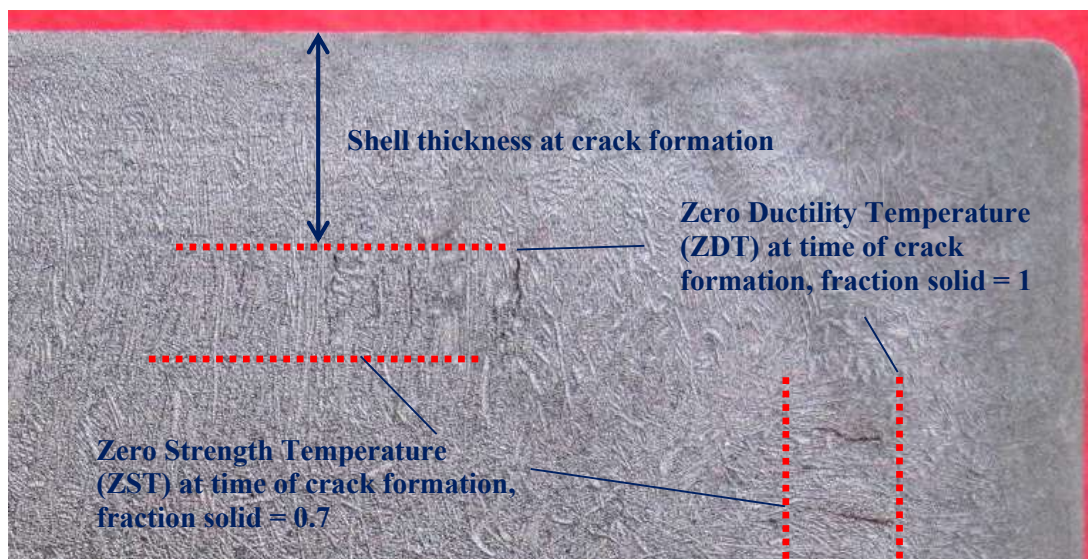

Figure 7. 150x150 mm billet showing typical internal cracks. See text for details.

Basically, this means that internal cracks occur when the fraction solid is between 1 and ~0.7. *Figure 6* shows that the difference between ZST and ZDT is greatly increased for hard cooling, because the solidus temperature is depressed, and highly segregated liquid remains between the dendrites down to very low temperatures (of course only under the assumption of the same liquid pool size, which might not be the case). If the complete steel chemistry would be considered in the calculations if would be seen that also S, P, and all other elements strongly segregate between dendrite arms making the cracking tendency far more severe for hard cooling. What makes the problem of cracking even worse is that the high cooling intensities applied during hard cooling also result in higher thermal stresses and strains, further aggravating the cracking problem.

The calculated fraction solid curve shown in *Figure 5* can thus directly be used together with the calculated temperature profiles of the cast billet shown in *Figure 4* to interpret the position in the continuous casting machine where the cracks are formed. This information is of great practical value for eliminating the internal cracking problem by optimizing casting parameters (balance between secondary cooling intensities of zones, adjust specific water volume, etc…), by improving maintenance (nozzle alignment, nozzle clogging, etc…) or improving the design of the continuous caster (longer secondary cooling zone, reduced gaps between secondary cooling zones, etc…).

6. Billet Solidification Microstructure for Different Solidification Rates

So, if hard cooling results in higher micro-segregation, makes the steel more susceptible to hot cracking and also results in higher thermal stresses and strains putting very high requirements on the design and maintenance of the continuous casting machine, why should anyone be interested in applying this technology?

Up to now we have only investigated micro-segregation that occurs between the secondary dendrite arms. This micro-segregation is not really a problem for downstream processing of the billet. The big problem is macro-segregation, that is found close to the centre. It is widely recognized that hard-cooling does in fact reduce this macro-segregation, however the mechanism by which this happens seems poorly understood. It is sometimes suggested that the higher cooling rate and steeper thermal gradients result in a finer branching dendrite microstructure at the solidification front that traps solutes and prevents them from being pushed ahead of the growing shell towards the centre of the billet.

To investigate this assumption, a multiple phase field simulation for the simplified C80D steel-grade investigated in this paper was set-up using the MICRESS simulation package that has already been applied to other continuous casting problems [11] [12]. The cooling rate and the temperature gradients in the billet are taken from the solidification simulation shown in *Figure 4* for a point 20 mm below the billet surface. All thermodynamic materials properties and the diffusion kinetics required for the phase field simulation are calculated using Thermo-Calc and are passed to MICRESS through the TQ programmers application interface [13] [14]. *Figure 8* compares the dendrite morphology for the thermal gradients obtained for hard cooling and soft cooling.
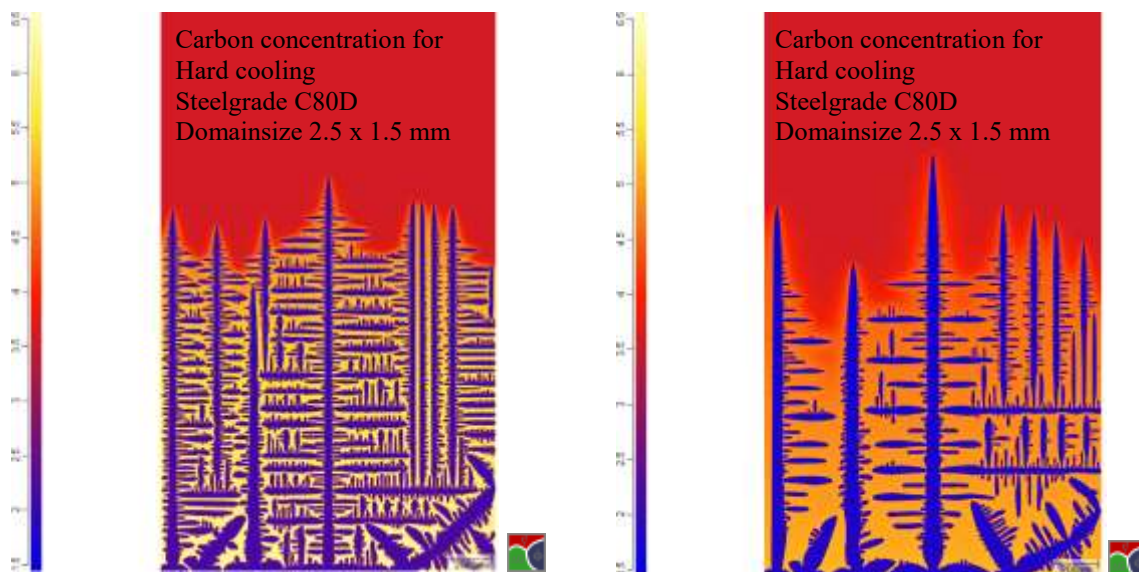

Figure 8. Solidification microstructure of C80D steel-grade with temperature gradient and cooling rate corresponding to hard cooling (left) and soft cooling (right).

Macro-segregation cannot be fully understood without considering the flow of liquid steel, in particular the suction effects induced by the volume shrinkage on final solidification resulting in the well-known V-segregation. Diffusion only takes place in the micro-meter range and is irrelevant. The phase field simulations clearly demonstrate the well-known finer dendrite microstructure that evolves when the thermal gradient and cooling rates are higher. This finer microstructure has a lower permeability for the liquid steel. Therefore the flow of highly segregated interdendritic melt towards the billet centre is obstructed and macrosegregation is reduced.

7. Conclusions and Outlook

This paper by no means has the ambition for an in-depth description of the billet solidification. The aim is to outline the linking together of readily available materials simulation tools, namely thermodynamic calculations, diffusion calculations, finite element solidification simulations and phase field modelling to elucidate a real-life industrial example from several angles in what could be considered an integrated computational materials engineering approach (ICME) [15]. All calculations are performed with state-of-the-art software packages and materials properties databases, but with many simplifications such as 2D calculations instead of 3D, strongly simplified steel chemistry, linearized thermal gradients, neglected fluid flow and gravity effects, no coupling between the models, etc… The simplifications have however been carefully chosen, so that all calculations still correctly capture the essence of the hard-cooling process. The next step is to expand and adapt the outlined models and apply them to the far more complex real-world industrial process.

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