Design of As-Cast Structures of Continuously Cast Steel Grades: Modeling and Prediction

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The prediction of the solidification structure by means of calculations and simulation programs is of great importance for controlling the quality of continuous casting (CC) semis. Plant components, different process control options, and the chemical composition of the as-cast product require optimized coordination of those factors to be able to set the optimum structure. As the simulation of temperature fields to predict the crater end during final solidification is already state of the art, the precise simulation of the solidification zones in CC semis is the important next step. Therefore, a circular arc caster is simulated with nucleation, grain growth, and sedimentation considered. The asymmetric as-cast structure is calculated with a good accuracy providing a good base for the implementation of microsegregation in the next development step.

1. Introduction

For the prediction and design of as-cast structures, it is important to distinguish between the different solidification structures, as in the end they influence the semis properties. The solidification conditions and the alloy itself influence solidification of steel, but the casting machine has an additional impact.

Online models that calculate the progressive solidification based on the heat transfer are used in steel plants, for example, to avoid whale formation or to determine the optimum position for applying soft reduction. For understanding the interaction of various phenomena and the micro- and macrostructural development in continuous casting (CC), many recent models combine several complex phenomena.1,2 These simulations may combine commercial software and own approaches. For modeling and calculation of the dendritic solidification structure, often a combination of temperature field and cellular automata or phase-field method is used. Otherwise, simply the shell thickness is derived from the temperature field as a measure of the solidification progress.3–10

The approach presented in this article incorporates a prediction of the solidification zones in a continuously casted slab based on a temperature field model considering the sedimentation of free grains without an additional microscale model for the microstructural evolution.

1.1. Solidification Structures

Dendritic structures can be divided in columnar and undirected grown, whereas the last category means as well-equiaxed dendrites as globulites (Figure 1). During dendritic solidification, the microsegregation gets captured between the dendritic arm spaces. As globulites have a round shape and no branches, this structure provides bigger coherent area. This leads to every solidification structure influencing the local hot ductility behavior of the material during casting among others.11–14

Consequently, it is important to characterize the difference between the solidification structures as in the end they influence the semis properties.

1.2. Sedimentation

In CC, which starts vertically and ends horizontally, the sedimentation of solid crystals and low-concentrated nuclei lead to a displacement of the residual melt and thus to the formation of an enriched area at the top of the slab. In turn, in the sedimented area, a wide cluster of segregation, the semimacrosegregation, can be found. The sedimentation has a significant effect on the solidification and segregation profile of slabs of circular arc and vertical bending plants.15–18

Figure 2 shows the schematic representation of a typical as-cast structure of a slab casted in a circular arc caster and two examples of real as-cast structures affected by sedimentation.

2. Modeling of the Solidification Zones in a CC Slab

The model introduced is an advancement of the temperature field model “SolSlab,” developed by Senk at the steel institute IEHK. The main objective is predicting the solidification zones in a circular arc slab caster. As an effect of gravity, free equiaxed and globular crystals can sink, and thus change the distribution of fraction solid $f_s$ and fraction liquid $f_l$ in the simulation cells. Therefore, not only the temperature field but also the...
development and change of the dendritic structure needs to be calculated in each time step of the solidification model. The final result of the simulation describes a quasistationary situation in the casting machine by calculating the entire temperature field incrementally along the casting direction.

The input data consists mainly of a digital twin of a simulated caster, and the enthalpy of the steel grade as well as the change of $f_s$ for an equilibrium solidification from Thermo-Calc, Figure 3.

2.1. Temperature Field

The temperature field inside the CC slab is a product of the different heat transfer mechanisms heat conduction $q_{\text{cond}}$, convection $q_{\text{conv}}$, and radiation $q_{\text{rad}}$, as shown in Equation (1)–(3).[19]

In each cooling zone of the casting machine, the respective heat transfer mechanism affecting the strand surface and has to be considered. Inside the strand, the heat is removed through conduction perpendicularly to the temperature gradient between overheated melt in the middle of the CC semi and the cooled...
surface.\cite{20} For a high accuracy especially of the temperature profile of the slab surface, each water-cooling nozzle and roll contact are included in the digital twin of the simulated caster.

\[ q_{\text{cond}} = -\lambda \frac{dT}{dx} \]  
\[ q_{\text{co}} = \alpha \times (T_{\text{surface}} - T_{\text{cooling water}}) \]  
\[ q_{\text{rad}} = A \times \varepsilon \times \sigma \times (T_{\text{surface}}^4 - T_{\text{surrounding}}^4) \]

where \( T \) is the temperature, \( \lambda \) is the thermal conductivity, \( x \) is the distance, \( \alpha \) is the heat transfer coefficient, \( A \) is the surface area, \( \varepsilon \) is the emissivity, and \( \sigma \) is the Boltzmann constant.

The temperature profile of the slab is calculated without implementation of the cooling of the narrow sides and the resulting solidification triangle. As the influence of the movement of the solid mass is to be observed in the simulation, the temperature field is simulated for the total thickness of the slab and not considered symmetrically for loose side and fixed side of the strand. As shown in Figure 4, the cells are calculated from both outer sides toward the slab center \( C_l \) starting at the loose side and proceeding with the fixed side. The cell in the slab center will not be considered until the heat transfer from both sides has been completely calculated, and thus is influenced by the temperature profile at loose side and fixed side.

### 2.2. Solidification Structure

#### 2.2.1. Nucleation

It is assumed that the nucleation starts with the temperature of the simulated cell dropping under the liquidus temperature \( T_{\text{liq}} \). The resulting fraction solid \( f_s \) in the time step where the nucleation starts is defined through data from Thermo-Calc. It has been defined that nuclei exist if this included data predicts \( f_s > 0 \).

#### 2.2.2. Dendritic Growth

For the growth of columnar dendrites, the assumption of the solidification front moving from the surface into the melt with the liquidus temperature is made. Thus, the speed of the solidification front \( v_{\text{columnar}} \) is proportional to the temperature difference \( \Delta T \) and depends on the diffusion coefficient \( D \) and the temperature gradient \( G \) over a distance \( x \) (Equation 4 and 5).\cite{21,22}

The resultant fraction solid \( f_{s,\text{columnar}} \) is imported from a Thermo-Calc file (Figure 3), and thus is always depending on the current temperature. The increase in \( f_{s,\text{columnar}} \) is used for the description of the columnar dendritic growth in direction of the slab center.

\[ v_{\text{columnar}} = G \times D \frac{dT}{\Delta T} \]  
\[ G = \frac{dT}{dx} \]

As equiaxed dendrites can move free in the melt, the solid fraction \( f_{s,\text{equiaxed}} \) can only be described using Thermo-Calc data in the initial simulation step. Afterward, the movement of the dendrites leads to a movement of the \( f_{s,\text{equiaxed}} \), which needs to be considered.

#### 2.2.3. Sedimentation

Particles with a minimum diameter \( d \) of 0.5 \( \mu m \) are able to sediment with a sinking rate directly proportional to the radius of the crystal. Stokes law can be used for the estimation of the sedimentation speed \( v_s \) according to Equation (6), given that the flow is laminar and the particles are sphere-shaped.\cite{16,23}

\[ v_s = \frac{d^2 \times g \times (\rho_p - \rho_f)}{18 \times \eta_f} \]

where \( g \) is the gravity, \( \rho_p \) the density of the particle, \( \rho_f \) the density of the fluid, and \( \eta_f \) the dynamic viscosity of the fluid.

In the simulation, the shape of the equiaxed dendrites is assumed to be spherical for simplification. The diameter of the spherical particles \( d \) in the individual simulation cell with a volume \( V_n \) is derived from \( f_{s,\text{equiaxed}} \) and a fixed number of nuclei \( N \) according to Equation (7).

\[ d = \sqrt[3]{\frac{6 \times (f_{s,\text{equiaxed}} \times V_n)}{N \times \pi}} = 2r_{\text{equiaxed}} \]

The sedimentation speed is now calculated depending on the radius of the equiaxed dendrites \( r_{\text{equiaxed}} \) and the solid fraction. Figure 5a shows that \( v_s \) increases with an increasing radius, but only until the total volume of sinking dendrites limits the sedimentation process. For \( f_s \geq 0.5 \) no free movement is allowed.\cite{24}

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**Figure 4.** Schematic representation of the simulation operation, with temperatures being first calculated from loose side and fixed side and last at the center of the slab.
Further, it is determined in the simulation into which the dendrites of the neighbor cell will move in the direction of the gravity and the position of the cell in the casting machine (Figure 5b).

On the basis of the successive calculations of the cell values in casting direction, the flow of the whole material in this direction is already included. As a consequence, the moving of the grains along the flow direction of the strand needs not to be considered separately in the model.

2.2.4. Columnar-to-Equiaxed Transition

The computational model for the distinction of the columnar-to-equiaxed transition (CET) is based on Hunt’s criterion.[25,26] In each simulation step, the solidification front is determined and a case distinction is made whether the $f_s$ ahead is exceeding 0.5. This value is used for the solidification front of the columnar dendrites because they dominate the solidification structure in the affected simulation cell. Below the value of 0.5 cannot, yet, be distinguished which dendritic structure will be decisive in that area. Figure 6 shows that at the loose side, the columnar dendrites can grow unimpeded, as the equiaxed dendrites sediment as described. The sedimented dendrites lead to a two-case scenario at the fixed side. Either $f_s < 0.5$ and the columnar growth strides onward (case A) or the high volume of solid crystals block the columnar front and the CET is identified (case B). Currently only terms for the columnar and the equiaxed areas are defined in the model, conditions for the beginning and the end of the transition zone are not defined yet.

3. Simulation Results of Solidification Zones in a CC Slab

Results are displayed for a slab, casted in a circular arc caster with a thickness of 350 mm. The real casting conditions like cooling intensity and casting velocity are implemented in the simulation. The results were verified with the cross section of a slab from the simulated cast. In the following, the calculations are shown for a nonalloyed steel with a carbon content of 0.5 wt%. The corresponding values of the steel properties and the simulation settings are shown in Table 1.
3.1. Temperature Field

Given that the cooling conditions at the loose and the fixed side of the strand are equal, the resulting temperature field is symmetrical in first instance (Figure 7a). Because the heat is extracted from the surface of the slab, the areas near the surface are colder at all times in the process than the areas further in the middle of the strand. Only with longer casting lengths, the temperatures from the center of the slab adjust to the temperatures on the surface. The temperature profiles at different distances from the slab surface (Figure 7b) show the effect of the cooling applied on the strand surface.

Directly beneath the surface, the consideration of each spray cooling nozzle, roll contact, and unimpacted surface leads to a constant alternation of cooling and reheating. Further away from the surface, the temperature loss is more uniform as the only heat transfer mechanism inside the strand is conduction and therefore the heat loss depends on the temperature difference to the neighbor simulation cell.

3.2. Solidification Structure

The advancement of the simulation included the sedimentation of equiaxed dendrites to predict the length of the solidification zones in the as-cast structure. To illustrate the effect of sedimentation on the development of the solid fraction during casting, \( f_s \) based on the symmetrical temperature field and \( f_s \) after implementation of the sedimentation criteria are shown in Figure 8.

According to the integrated data, the strand is completely solidified at a casting length of \( \approx 21 \) m. From a casting length of \( \approx 13 \) m, all temperature values are already below the liquidus temperature, so that the slab only consists of a heterogeneous area and completely solidified areas at the surfaces.

The consideration of sedimentation changes the distribution of the solid fraction over the whole slab thickness. In the equiaxed zone, the dendrites move and thus the fraction solid is recalculated. In the next simulation step, the movement of the equiaxed crystals consequently results in a change of the temperature field. Therefore, the recalculation of the fraction solid follows a calculation of the heat exchange between the cells. The new \( f_s \) distribution is shown in Figure 8b from 144 to 293 mm of the slab thickness, which reflects the area of undirected solidification. An unsteady distribution of the solid fraction within the undirected area results from the sinking of solid mass in direction of the gravity. The rapid change of \( f_s \) at 144 mm is due to the fact that the origin and growth of undirected nuclei still continues in front of the columnar dendrites. The generated grains sink down until the volume fraction of the solid phase in the direction toward the fixed side is too high and the sedimentation stops. Because of the undercooling in the area close to the columnar dendrites, the grains grow more quickly which is resulting in the discontinuous transition of \( f_s \).

At the shown vertical lines, which represent the transition of the structural zones and thus the CET, the proportion of the solid phase increases faster compared with the center region. A growing distance of the lines representing constant \( f_s \) values hints to a slower increase.

| Property              | Unit      | Value  | Setting            | Unit    | Value  |
|-----------------------|-----------|--------|--------------------|---------|--------|
| Liquidus temperature  | K         | 1751.4 | Slab cross-section | mm      | 2000 × 350 |
| Solidus temperature   | K         | 1707.8 | Casting speed      | m min⁻¹ | 0.65   |
| Specific heat capacity| J/(kg · K)⁻¹ | 650    | Superheat          | K       | 25     |

Table 1. Steel properties and the settings used in the performed simulation.

Figure 7. a) Calculated symmetrical temperature field depending on the casting length over the height of the slab and b) temperature progression over the casting length at different distances from the slab surface.
The exact distribution of the solid phase is shown in Figure 8b, in addition, in Figure 9a, distinction is made between the structural zones of directed (green) and undirected (red) solidification. The area where the melt cannot be classified to a morphology, yet, so the area which is still completely liquid, is shown in blue. If there is a first solid component generated in the area, a structure is assigned to the simulation cell according to the criteria described in Section 2.2. At the end of solidification, there is a longer-directed zone on the loose side of the slab than on the fixed side. The equiaxed zone is not located symmetrical in the center of the slab and can mostly be seen on the fixed side. In addition to dividing the structure zones at the end of solidification, the image also shows the casting length at which the change between the solidification morphologies takes place. It can be clearly seen that the CET zone on the fixed side forms earlier in the process than on the loose side.

4. Validation of the Simulation

The simulation results are validated with a slab casted in the modeled caster under casting conditions used for the calculation. The compared dimensions of the identified solidification zones are shown in Table 2. The length of the columnar dendritic zone is about 14% shorter than measured in the as-cast slab. This leads to the conclusion, that the criteria relevant for the geometrical aspect of sedimentation are implemented correctly.

The deviation is believed to result out of the solidification parameters used. The simulation is based on an equilibrium solidification which is not the case in real slab casting. Solidification phenomena like microsegregation are not yet considered in this version of the program.

5. Conclusions

With the developed model a further step was taken with the aim of predicting the as-cast structures during the casting process. The program is based on the stepwise calculation of the temperature profile along the casting length. The growth conditions for the columnar and equiaxed dendrites have been included in the extended model, as well as the sedimentation of the free grains. Thus, a first approximation of the development of the structures with given casting conditions can be calculated with the described model.

| Table 2. Comparison of simulation results and the real as-cast structure. |
| --- | --- | --- |
| | Loose side | Fixed side |
| Length of columnar zone (calculated) [mm] | 147 | 61 |
| Length of columnar zone (as-cast) [mm] | 170 | 71 |
| Relative deviation [%] | 13.5 | 14.1 |
The implementation of microsegregation and thus an extended the temperature range where a liquid phase exists, is expected to enhance the predictions accuracy in the near future.

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Conflict of Interest

The authors declare no conflict of interest.

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