Columnar-equiaxed transition in continuous casting based on a micro-macro solidification model with long-range solutal mixing

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Abstract. A novel model is proposed to describe the columnar to equiaxed transition (CET) in continuous casting. The model bases on Rappaz and Thevoz’s solute diffusion model for equiaxed dendritic growth, combined with a 1-Dimensional solidification model normal to the slab surface. The unique feature of the proposed model is the combination with a mixing term between interdendritic and extradendritic melt, representing long-range solutal mixing by convection. The model can also be applied to predict equiaxed to columnar transition (ECT), i.e. the chill zone thickness. The model consists of modules such as nucleation, growth kinetics, solute and heat balance, and a solute mixing module. Nucleation is considered with a fixed nucleation undercooling. The growth kinetics of the dendrites are treated according to the LGK model. A finite difference scheme is employed for solving 1-Dimensional heat transfer equations and finally, volume averaged solute balance equations are solved in a staggered scheme. Mixing of inter- and extradendritic liquid is, as a first step, treated ideally fast. When applied to Fe-C binary system with the thermo-physical properties obtained from literature and CALPHAD simulations, the model successfully predicts recalescence, phase fraction evolution, and concentration profiles in different phases. Realistic boundary conditions of the continuous casting process are obtained from macroscopic FEM simulation.

1. Introduction
Continuous casting technology is the most economical way of steel making and currently it is responsible for more than 95% of world's steel production [1]. A typical solidification structure of a steel grade contains both columnar and equiaxed dendrites. At microstructural scale, the decisive factor that defines the homogeneity of a steel grade is the amount of equiaxed dendritic region [2]. Hence, one of the primary objectives of continuous casting is to reduce the amount of columnar dendritic region and optimize the equiaxed crystal region. In this regard, numerous studies have been made to predict and control columnar to equiaxed transition which determines the amount of equiaxed dendritic region. However, due to numerous mechanisms that are active at various time and length scales, computational modelling of CET has still remained as a challenging task [3]. With the present model, we aim to propose a novel CET mechanism by considering long-range solutal mixing which arises due to convection.
1.1. CET Models

Over the past decades, computer modelling has played a significant role in understanding CET under various solidification conditions. Although CET and the factors influencing the transformation are qualitatively well understood, simulation models have not reached a stage to make quantitative predictions. This is mainly due to the complexities in the interaction mechanisms [3]. At present, numerous models are available in the literature which offer both direct and indirect predictions of CET and related microstructural evolution features. However, the transformation mechanisms employed in these models differ a lot from each other thereby making it difficult for the beginners who want to understand the phenomena of CET [4].

Witzke et al. [5] modelled solutal and temperature distributions ahead of a columnar front and suggested that CET requires two conditions. First, the liquid metal ahead of the columnar front should reach sufficient degree of solutal undercooling and second, the volume of the undercooled liquid zone should be high enough. According to them, these two are the necessary conditions for nucleation of new equiaxed crystals which hinder the growth of columnar front. Further, Lipton et al. [6] have also suggested similar mechanism where they proposed that CET is mainly governed by the undercooling of the columnar interface and width of the undercooled boundary layer at the columnar interface.

In 1986, based on the extended volume fraction of equiaxed grains, Hunt proposed a widely accepted criterion for CET in 1D solidification [7]. He argued that CET happens if the volume fraction of grains in the undercooled melt ahead of the columnar front is higher than 0.49. However, the value of 0.49 is selected purely on geometrical considerations and lacks a strong physical explanation.

Wang and Beckermann [8, 9] proposed a novel technique to predict CET under the conditions of diffusion driven dendritic growth solidification. The model equations are derived by following multiphase approach in which each control volume is assumed to be consisting of three phases, solid, interdendritic liquid and extradendritic liquid. However, they have also employed mechanical blocking criterion to predict CET.

Further, to eliminate the usage of mechanical blocking criterion, Martorano et al. [10] proposed a new mechanism, where they took solutal interactions between equiaxed grains into account. They have implemented their model for different nucleation densities and found that CET does not always occur at 0.49 grain volume fraction. For the case of higher nucleation density, CET occurred at much lower volume fraction of grains whereas for the case of lower nucleation density, CET is delayed.

Owing to these differences in proposed mechanisms and complexities associated with implementing them at the realistic macro scale, most of the CET models at industrial scale are still relying on the fundamental Hunt’s model, even though there was no strong experimental validation supporting it.

1.2. Objectives of the current model

The objectives of the present model are multifold. First, to develop a 1-D numerical simulation model which can predict both CET and chill zone thickness. Second, to propose a new CET mechanism which bases on tracking the solute undercooling ahead of the columnar front. Third, to include the effects of long range solutal mixing in the solidification model. And finally, to enable direct coupling of temperature data obtained from industrial scale macro simulation models to the microscopic solute distribution equations so that the model can make effective predictions based on the actual process conditions.

2. Volume averaged solidification model in 1-D

The system under investigation is shown in figure 1. A slab of uniform thickness produced by continuous casting technique is considered. Due to symmetry of the slab geometry and applied boundary conditions, a quarter of the slab is generally sufficient for macroscopic modelling (see figure 1(a)). Further, due to uniform cooling conditions on the surface of the strand, a 1-D line from surface to the centre is taken as the system for microstructural investigation (see the red line in figure 1(a)). The outer surface is subjected to convective cooling and adiabatic heat transfer conditions are applied at the centre of the
slab. The arrow (blue colour) represents the direction of pulling of the slab from mould to the secondary rollers.

The solute distribution is treated according to Rappaz and Thevoz’s solute diffusion model [11, 12]. As shown in figure 1(b), each grain, irrespective of columnar or equiaxed dendritic microstructure, consists of 3 phases: solid dendrites (phase s), interdendritic liquid (phase d) and extradendritic liquid (phase l). The solid dendrites along with the interdendritic liquid trapped within the dendritic arms is termed as ‘grain’ (phase g). The two liquid phases, ‘d’ and ‘l’ are separated by a dendritic envelope due to differences in their interfacial length scales. Hence, dendrite envelope is defined as an interface that separates interdendritic and extradendritic liquid phases. Further, key assumptions of the model include, local equilibrium at the solid-liquid interface, finite diffusion of solute from interdendritic to extra dendritic phase and no diffusion of the solute in the solid phase. Also, peritectic reaction is not modelled and the initial solidification of delta phase and subsequent gamma phase are treated as uniform solid phase.

In each control volume, first the heat diffusion equation is solved to get the nodal temperatures. Based on the nodal temperatures, solute concentrations are obtained from linear phase diagram. Nucleation is assumed to happen instantaneously at a nucleation undercooling temperature and the growth kinetics of the envelope is treated according to LGK model [13]. Finally, based on the equations adopted from Wang and Beckermann’s model [8, 9], the solute balance is performed in each phase. The novel feature of the present model is consideration of effects of macrosegregation, which is treated with a solute mixing module explained in detailed in the corresponding section.

\[
\rho C_p \frac{dT}{dt} - L \frac{df_s}{dt} = \lambda \nabla^2 (T). \tag{1}
\]

**Figure 1:** (a) Schematic representation of quarter of a strand (slab), red colour line is highlighting the 1D-system under investigation. (b) Solidification system with boundary conditions. Convective boundary conditions are applied on left boundary and adiabatic heat transfer is applied on the right-hand boundary. \(T_E, T_c, T_L\) are temperatures corresponding to eutectic, columnar front and liquidus point. \(\Delta T_n\) is nucleation undercooling. (figure 1(b) is based on figure 1 in [8, 9])

**2.1. Model governing equations**

Based on the volume conservation approach, Wang and Beckermann developed the governing equations for heat and mass balance in all the existing phases. Since the detailed explanation for all the equations are given in the original paper [8, 9], they are only summarized here.

The temperature distribution is calculated according to the following heat conduction equation with latent heat and appropriate boundary conditions.

\[
\rho C_p \frac{dT}{dt} - L \frac{df_s}{dt} = \lambda \nabla^2 (T). \tag{1}
\]
Solute balance in the solid phase (phase ‘s’) neglecting the back diffusion, is calculated from,
\[ \frac{d}{dt} (f_s C_{avg}) = k C_i \frac{df_s}{dt}. \]  
(2)

Solute Balance in interdendritic liquid (phase ‘d’) with infinite mixing is calculated from,
\[ C_i (k - 1) \frac{df_s}{dt} + f_d \frac{dC_i}{dt} = - \frac{S e^{diq}}{\delta} (C_i - C_{liq}); \ C_i^* = \frac{T-T_{iron}}{m_{liq}}. \]  
(3)

Solute balance in extradendritic liquid (phase ‘l’) with finite diffusion, is calculated from,
\[ \frac{d}{dt} (f_l C_l) = C_i^* \frac{df_l}{dt} + \frac{S e}{\delta} D_{liq} (C_i^* - C_{liq}). \]  
(4)

Further, the interrelationship between the three phases in each control volume is given as follows.
\[ f_s + f_d + f_l = 1; \ f_g = f_s + f_d; \ f_l = 1 - f_g; \ \frac{df_g}{dt} = - \frac{df_l}{dt} = S e V_{tip}, \]  
(5)

where \( p \) is density, \( C_p \) is heat capacity, \( L \) is latent heat, \( \lambda \) is heat conductivity (taken as a constant), \( f_s, f_d, f_g, f_i \) are volume fractions of solid, interdendritic liquid, grain and extradendritic liquid respectively, \( C_{avg}, C_i, C_l \) are the average solute concentrations in solid, interdendritic liquid and extradendritic liquid of each control volume. \( C_{liq} \) is the nominal composition of solute in the remaining liquid metal which is obtained from the solute mixing module. Further, \( k \) is the equilibrium partition coefficient, \( m_{liq} \) is the slope of the liquidus line, \( D_{liq} \) is the diffusion coefficient in the liquid phase, \( \delta \) is the diffusion length, \( S_e \) is the envelope surface area concentration and \( V_{tip} \) is the dendrite tip velocity.

With an assumption of spherical dendrite, \( S_e \) and \( R_g \) are calculated from,
\[ S_e = \frac{3\pi R_g^2}{R_{avg}^3}; \ R_g = (f_g^{1/3}) R_{avg}, \]  
(6)

where, \( R_g \) is the radius of the grain or envelope and \( R_{avg} \) is the average spacing between dendrite envelopes.

As stated earlier, LGK kinetics is employed to calculate \( V_{tip} \). Hence, \( V_{tip} \) is given by,
\[ V_{tip} = \frac{D_{liq} m_{liq} (k-1) C_i^*}{\pi^2 \tau} \left[ 0.4567 \left( \frac{\alpha}{1-\alpha} \right)^{1.195} \right]^2; \ \Omega = \frac{C_i^* - C_{liq}^*}{C_i^* (1-k)} \]  
(7)

where \( \tau \) is the Gibbs-Thomson coefficient and \( \Omega \) is a dimensionless quantity known as the supersaturation.

Note that the equation used to calculate supersaturation \( \Omega \) is different from the previous CET models. In their original model, Rappaz and Thevoz \([11, 12]\) used initial alloy concentration \( C_0 \) to calculate supersaturation ahead of the dendritic front. Wang and Beckermann \([8, 9]\) also used \( C_0 \), at least to calculate supersaturation in columnar dendritic region. Hence, they had to use mechanical blocking criterion to predict CET. Later, Martorano et al. \([10]\) modified the equation by replacing \( C_0 \) with \( C_i \) for both columnar and equiaxed growth. However, the effects of long-range solute mixing have not been considered in any of the existing analytical models. Hence, in the present model, a solute mixing module is developed to incorporate such effects and resulting macrosegregation.

### 2.2. Solute enrichment due to melt convection

Due to the complexities associated with fluid interactions, most of the existing CET models have neglected the effects of the turbulence and macrosegregation. Thus, the predictions for CET and other microstructural quantities obtained from such models are independent of melt convection effects. However, fluid flow in continuous casting process, especially in the mold part, has a very strong influence on the solidification microstructure of the slab. To bridge this gap, the present model aims to demonstrate a way to include the effects of a macrosegregation through a simple and easy to implement approach.

The key idea behind the proposed solute enrichment module is that, the nominal solute concentration i.e. the concentration of the solute available at the start of the solidification increases as the solidification proceeds from surface to the centre of the slab. Due to solute transport at the macro scale resulting from the turbulence inside the melt, the liquid metal away from the outer surface solidifies with higher nominal solute concentrations. In the present model, it is realized by allowing infinite mixing of the
amount of solute available in extradendritic liquid phase of each control volume. This results in uniform solute concentration in the far away liquid, $C_{liq}^f$.

Having known the fraction of liquid and solute concentration in extradendritic liquid in each control volume, solute enrichment due to mixing is calculated from, 

$$C_{liq}^t = \frac{\sum_{i=0}^{N} f_i C_i}{\sum_{i=0}^{N} f_i},$$

which is of course an extreme, limiting case. Here, $N$ is the total number of control volumes or nodes in the system, $f_i$ is the fraction of liquid in each control volume and $C_i$ is the solute concentration in extradendritic liquid in each control volume. Further, $C_{liq}^f$ is calculated as long as the solidification front reaches the centre of the slab model.

2.3. The CET mechanism

A typical microstructure of a steel slab contains three dendritic regions, chill zone near to the cooling surface (outer equiaxed) followed by columnar dendritic, and globulatic region close to the centre (inner equiaxed). Also, we know that nucleation and growth of equiaxed grains require the melt to be undercooled. From this information, we can conclude that, during the solidification, the local undercooling in outer and inner equiaxed regions must be higher than nucleation undercooling and that of the columnar region should be below the nucleation undercooling. Figure 3 schematically explains the same. The blue curve which represents the amount of solute undercooling ahead of the solidification front is seen to decreasing from outer surface and again increasing towards the centre of the slab.

According to Kurz et al. [2], the amount of undercooling ahead of the solidification is resulting from solute redistribution due to diffusion and it has quadratic relationship with the front velocity. Further, at low velocity regimes, the undercooling is driven by temperature gradients in the liquid metal (refer to figure 2). However, at the realistic scale, the temperature gradients in the liquid metal are almost negligible hence it alone cannot explain the rise of undercooling towards the centre of the slab. Hence, in the present model, we propose that the rise in local undercooling towards the centre of the slab is not only due to temperature gradient in the liquid metal but also due to solute enrichment that results from both diffusion and macroscopic solute mixing.

By assuming ideal solute mixing, we calculate average solute concentration in the whole liquid phase i.e. $C_{liq}^f$, and this concentration is used to calculate supersaturation and local undercooling. As shown in figure 3, by comparing the local undercooling with nucleation undercooling the model predicts both chill zone thickness and CET.

![Figure 2: The equilibrium liquidus temperature and local temperature profile ahead of a dendritic front, after [2]](image2)

![Figure 3: Schematic representation of proposed CET mechanism. $\Delta T_c$ and $\Delta T_N$ are solutal and nucleation undercoolings respectively.](image3)
2.4. Model implementation

A numerical solution is obtained by discretizing the heat and mass balance equations and solving them with a finite difference method. The heat balance equation is solved with implicit finite difference scheme. Cellular automaton based front tracking algorithm is employed to track the solidification front. Once a control volume is activated for solidification, $C_l^i$ is obtained from the liquidus line of a binary equilibrium phase diagram. Then the quantities such as $V_{tip}$, $f_g$, $f_i$, and $C_l$ are obtained by iteratively solving the corresponding equations. Finally, equations 1 and 3 are solved simultaneously to obtain both $T$ and $f_g$. Knowing volume fractions and solute concentrations of each phase in every control volume, all the remaining quantities are calculated.

3. Results

The volume averaged solidification model coupled with long-range solute mixing is implemented to predict CET, chill zone thickness (ECT) and other microstructural evolution features of Fe-0.15 wt% C alloy. Thermo-physical properties of the binary alloy are as follows: liquidus temperature, $T_{liq} = 1791\,K$, eutectic Temperature, $T_{eut} = 1400\,K$, density of the liquid metal, $\rho = 7440 \, kg/m^3$, specific heat, $C_p = 720 \, J/kg/K$, heat conductivity, $\lambda = 30 \, W/m-K$, melting point of pure iron $T_{mp} = 1809\,K$, slope of the liquidus line $m_{liq} = -90 \, K/wt\%$, equilibrium partition coefficient $K = 0.36$, diffusion constant of the liquid $D_{liq} = 2.0 \times 10^{-6} \, m^2/s$, gibbs Thomson coefficient $\tau = 1.35 \times 10^{-7} \, Km$, and latent heat $L = 2.71 \times 10^5 \, J/m^3$.

A slab of half thickness 100 mm is taken as the 1-Dimensional linear system and is divided into number of control volumes. The initial temperature of the liquid metal was uniform with a superheat of 10 K. Adiabatic boundary conditions are applied at the centre of the slab (right boundary) and constant cooling boundary conditions are applied at the cooling surface (left boundary) by $q = h(T - T_{in})$ where the heat transfer coefficient was $h = 2000 \, W/m^2-K$ and ambient temperature $T_{in} = 300\,K$. Fitting parameters such as nucleation density and nucleation undercooling are taken as follows: nucleation density $n = 2.39 \times 10^8 \, m^{-3}$ and nucleation undercooling $\Delta T_p = 2.5\,K$. Fragmentation of dendrite tips due to solutal mixing is considered indirectly by choosing high volume of nucleation grain density.

First, the results obtained for the evolution of all the involved phases in a control volume are presented in figure 4. The associated cooling curve (T), liquidus temperature and nucleation temperatures are also shown in the same figure. As it can be seen in the figure, at the start of solidification, the control volume is completely in liquid state i.e. $f_l = 1$ and $f_s = f_d = f_g = 0$. As the temperature decreases due to cooling, dendritic growth proceeds and the solid phase starts to form out of the liquid. Hence $f_g$ and $f_i$ increase and $f_l$ decreases. The interdendritic liquid phase, $f_d$, raises initially with $f_g$ until the latter reaches its full volume fraction i.e. until $f_g = 1$. Once the grain growth stops, the solid phase continues to grow from the remaining interdendritic liquid. Further, the model can also calculate the solidification time and metallurgical length of the slab which are of industrial interest. For the chosen cooling rate and process parameters, the model predicts that a slab of thickness 200mm takes about 700 seconds for complete solidification.
Finally, figure 5 presents the results obtained for dendrite tip velocity, solute undercooling and nominal solute concentration observed in each control volume. From the figure, it can be seen that, when the solute mixing is active, the undercooling is decreasing from the cooling surface and again increasing towards the centre of the slab, whereas in the absence of solute mixing, the undercooling does not rise towards the centre. This change in slope undercooling in the first case, is attributed to the solute enrichment, resulting from macroscopic solute mixing. As solute undercooling is a function of both dendrite tip velocity and nominal solute concentration, it continued to decrease until the drop in the tip velocity is significant. Once the drop in the tip velocity has become relatively insignificant, solute undercooling continued to rise due to increase in solute concentration. By comparing the solute undercooling observed in each control volume with the pre-defined nucleation undercooling, one can easily identify the three dendritic regions, i.e. chill zone, columnar dendritic and inner equiaxed regions. In both chill zone and inner equiaxed regions, the solute undercooling is higher than nucleation undercooling, whereas in columnar dendritic region, the nucleation undercooling is higher than solute undercooling. For the chosen process parameters and nucleation undercooling of 2.5 K, the model predicts a chill zone thickness of 6 mm and CET at around 75 mm from the surface. The model is further validated for different nucleation density and nucleation undercooling values and the results are found to be satisfactory.

Figure 5. Maximum dendrite tip velocity and solute undercooling observed in each control volume. Nominal solute concentration of the control volumes and nucleation undercooling is also shown.

3.1. Results obtained for temperature data generated from the FE simulation model
The model setup enables direct coupling of temperature data obtained from macroscopic FE simulation models. To validate the functioning and applicability of the current model for the same purpose, it is implemented with temperature data obtained from a 3-Dimensional FE simulation model developed by thyssenkrupp steel Europe AG. The macroscopic FE simulation model calculates the temperature distribution in the strand shell with realistic process parameters and boundary conditions.

The temperature data is generated for a low carbon steel slab of 140 mm half thickness and of 0.15 wt% C carbon composition. The thermo-physical parameters are adopted accordingly. To calculate the chill zone thickness and CET, nodal temperatures along the half thickness of the slab, as represented by a straight line in figure 1(a) are considered. Owing to the massive size of the actual slab casting, the nodal spacing and time steps used in the FE simulation are bigger than those suitable for microstructural
simulation. Hence linear interpolation is used to obtain the temperatures as per the grid spacing and time step requirement of the present numerical model.

For a nucleation density of $2.39 \times 10^8 \text{ m}^{-3}$ and nucleation undercooling of 3 K, the model is able to qualitatively predict solute concentration profiles in both solid and liquid phases and predicts a chill zone thickness of 3 mm and CET at 75-80 mm from the cooling surface. These results are compared with an etched section of the corresponding steel slabs and the location of CET is found to be in reasonable agreement.

4. Discussion
The model predictions for CET are comparatively in good agreement with the literature and experimental observations available for similar grades [14]. However, the results obtained for chill zone thickness are not satisfactory. Since the chill zone thickness is strongly influenced by the initial cooling rate and available nucleation density, the observed discrepancy is likely to be a mere artefact of the chosen boundary conditions. Further, the mixing algorithm used in the present model is based on ideal mixing which is the extreme case of mixing. In reality, the fluid flow during the solidification of continuous casting of steels is driven by numerous factors ranging from electromagnetic forces, slab geometry, gravity, and turbulences. To be able to make quantitative predictions, the model needs improvements in two key areas. First, the mixing algorithm should be improved by taking reference from fluid simulations and second, the model should be extended to multi component alloy system.

5. Conclusion
Taking macroscopic solute mixing into consideration, a numerical model is proposed to predict both chill zone thickness and CET. The numerical model is developed based on the solute diffusion equations derived from volume averaged technique and the effects of macrosegregation are included through ideal solute mixing. When applied to Fe-C binary system, the model predictions obtained for temperature distribution, dendrite tip velocity, solute concentrations, and solute undercooling were in accordance with the fundamental understanding of solidification in steel. Additionally, the model is also tested for temperature data obtained from an industrial macroscopic FE simulation model. The results obtained have proved that the model can effectively predict CET for a given binary composition and process parameters. However, in order to make quantitative predictions and to compare the model results to actual casting microstructure, further improvement of solute mixing module is required.

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