Mathematical modelling of morphological transition and spot segregation in continuously-cast high carbon steel billets

Suryanaman Chaube
TCS Research,
TCS Ltd.,
Pune, India
Email: suryanaman.chaube@tcs.com

Abstract: In this work, the columnar-to-equiaxed transition (CET) and spot segregation phenomena in continuously-cast (CC) high carbon steel billets are investigated. Casting process is simulated for a 125 mm × 125 mm billet using a macroscopic thermal model. An empirical correlation, depicting the effect of melt temperature on heterogeneous nuclei density, is incorporated in the CET model to account for a more realistic variation of CET with melt superheat. A parametric study is also performed to see the influence of casting speed on CET and explore its theoretical limit for plant operation. The model is sufficiently general and can be utilised for different caster designs and processing conditions. Additionally, an attempt is made to estimate the degree of solute segregation in small spots along the billet centreline using a simple microsegregation model. The model predictions are compared with experimental observations on CC high-carbon steel billets and the results are encouraging.

Keywords: continuous casting; columnar-to-equiaxed; billet; high carbon; morphology; spot segregation.


Biographical notes: Suryanaman Chaube is a researcher at the TRDDC, Tata Consultancy Services Ltd., Pune. He completed his Bachelor and Master’s in Metallurgical and Materials Engineering from the Indian Institute of Technology, Madras in 2013. His recent publications include a research article on modelling casting solidification in Trans. IIM journal and abstracts in two conference proceedings. His major research interests are solidification, heat transfer in manufacturing processes, integrated computational materials engineering (ICME) and multiscale modelling.

1 Introduction
The recent advances in continuous casting (CC) technology and growing demands for high quality steel have engendered a need to address the challenges of increasing productivity and quality while reducing production cost in steel plants. This requires a careful optimisation of the operational parameters during different stages of the casting process as well as improvement in the whole CC process chain.

CC process, whereby molten metal gets solidified into semi-finished products, involves a complex series of parallel phenomena including heat and mass transfer processes, solidification, phase transformations, etc. The quality of the cast product is directly linked with the cooling intensity of the product during solidification in different zones of a caster. Modelling of CC solidification, therefore, has received considerable attention in the recent past. In particular, a lot of effort has gone into modelling of columnar-to-equiaxed morphological transition (CET) due to its high relevance in industrial application. A higher fraction of columnar dendrites makes a continuously cast billet more sensitive to cracking and increases the severity of centre-line segregation (CLS) (Ghosh, 2001). It can also lead to inhomogeneity in inclusion distribution, which has a sizeable effect on downstream processes such as rolling and fatigue behaviour of finished products under service conditions (Gupta et al., 2015). In practice, the equiaxed zone ratio can be increased by adjusting the process parameters such as the casting speed, tundish superheat, and the spray cooling conditions; or by means of electromagnetic stirring in order to increase the local number density of equiaxed grains. However, for exercising greater flexibility in customising the CC parameters with an aim of reducing internal defects, it becomes important to analyse the morphology using a predictive modelling framework.

There have been numerous theoretical and experimental investigations on modelling columnar grain growth in the melt (Bilioni and Chalmers, 1968; Chalmers, 1963, 1964; Morando et al., 1970; Walton and Chalmers, 1959). A
Mathematical modelling of morphological transition and spot segregation in continuously-cast high carbon steel

A comprehensive analysis of CET, however, was first presented by Hunt (1984) who analytically derived a critical gradient condition for fully-equiaxed growth. The models subsequently proposed factored in effects of nucleation, thermal undercooling and solute diffusion in the melt (Dong and Lee, 2005; Flood and Hunt, 1987; Martorano and Biscuola, 2009). These models were based on a mechanical blocking criterion, wherein, the CET was assumed to occur when the volume fraction of equiaxed grains at the columnar front reached a critical value. Subsequently, volume-averaged multi-phase models were formulated (Beckermann and Wang, 1995; Ludwig and Wu, 2005; Noeppel et al., 2009) to model transport phenomena on the scale of an entire casting. Also, meso-scale techniques to simulate the unsteady growth of multiple equiaxed dendritic grains into supercooled melts were developed. Examples are the cellular-automaton finite-element (CAFE) model (Gandin and Rappaz, 1994) or the front-tracking models (Steinbach et al., 1999; Delaleau et al., 2010). To further improve the accuracy of CET predictions, complex multi-phase formulations came up that modelled interactions between columnar and equiaxed dendrites through a solutal blocking mechanism (Jung et al., 2009; Martorano et al., 2003; Wang and Beckermann, 1994). Since both types of mechanisms yield negligible variations in CET predictions (Martorano and Biscuola, 2009), Hunt’s model can suitably be used owing to its easy adoption in macroscopic thermal models.

In the present investigation, a computational study of CET – based on simplified Hunt’s criterion – is performed and validated for a CC high-carbon steel billet (125 mm × 125 mm). Available data (Shamsi and Ajmani, 2010) for CC1 billet caster (Tata Steel, Jamshedpur) is used to predict shell thickness profile, columnar front velocity, thermal gradient and CET with the progress of solidification. For better CET predictions, a superheat linked dependency of the number density of effective nuclei – that grow into equiaxed grains – is incorporated into the model through an exponential decay of Hunt’s nucleation parameter $N_0$ (Chaube et al., 2015). With this treatment, the results show a much stronger dependence of CET with superheat even when the thermal gradients and growth velocities are insubstantially modified. A parametric study is carried out to assess the influence of casting speed and melt superheat on CET – as these parameters directly influence the metallurgical length and solidified shell thickness along the caster length.

Additionally, localised spot-segregation near billet centreline is modelled in this work for three species – C, S and Mn. Segregation is important as it leads to non-equilibrium phases, cracks and other problems which degrade the mechanical properties of the final product. Macrosegregation, which arises form large-scale fluid flow, is very complex and among many other things, depends on the solidification morphology and accurate prediction of microsegregation. A special case of microsegregation during casting operation is the formation of small segregation spots. These spots form along the centre-line due to the local entrapment of solute-enriched liquid drops among the last-solidifying dendrites. While simple segregation models cannot predict macrosegregation during continuous steel casting, they have been successfully employed to get reasonable estimates of centre-line spot segregation (Matsumiya et al., 1984; Tsuchida et al., 1984), which is an important quality parameter. In this analysis, a simple but accurate microsegregation model (Won and Thomas, 2001) is used that considers the effects of multiple components and dendritic coarsening during solidification and is explained in detail in Section 2. Obtained segregation ratios for the considered species are compared with the experimental findings of Choudhary and Ganguly (2007) and there is a good quantitative match.

2 Mathematical description of model

The coupled numerical model presented in this work calculates the solidification parameters to determine the morphology as well as segregation characteristics of CC billets and is described below. Dimensions of the caster are given in Table 1. Figure 1 represents a process flow-chart of the model.

Figure 1 Flowchart of the combined thermal and spot segregation model
Table 1  
Caster geometry used in the present computations  

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Tata steel, CCI</th>
</tr>
</thead>
<tbody>
<tr>
<td>Section size</td>
<td>0.125 m × 0.125 m</td>
</tr>
<tr>
<td>Mould length (m)</td>
<td>0.741</td>
</tr>
<tr>
<td>Spray zone length</td>
<td></td>
</tr>
<tr>
<td>Spray ring (m)</td>
<td>0.431</td>
</tr>
<tr>
<td>1A–1B</td>
<td>1.121</td>
</tr>
<tr>
<td>2A–2B</td>
<td>3.874</td>
</tr>
<tr>
<td>Length at cut (m)</td>
<td>15.9</td>
</tr>
</tbody>
</table>

2.1 Solidification morphology

The mathematical formulation of solidification model to predict the temperature distribution and the solid shell profile is based on Fourier’s equation of heat conduction in unsteady state. The simulation domain for this part of the model is a transverse slice which moves down through the mould and spray regions at the casting speed, as shown in Figure 2. Though the caster has a curved shape, it is assumed to be vertical and of fixed dimension throughout the process. This assumption doesn’t significantly affect the shell thickness and temperature profiles (Shamsi and Ajmani, 2010). Considering the symmetry of heat flow in billet, only a quarter section of the slice is modelled. Also, thermal gradient in the axial direction is not relevant for modelling growth of columnar front and CET and is ignored. In order to account for bulk convection by the submerged entry nozzle, an enhanced thermal conductivity in the mush is considered using the solid-liquid coexisting zone model (Shibata et al., 2006).

Figure 2  
Schematic of the modelling domain (see online version for colours)

2.1.1 Heat conduction equation

The temperature evolution in the solidifying steel shell is through a continuous solidification process and can be described by the following two-dimensional heat transfer equation:

\[
\frac{\partial}{\partial t}(\rho C_p T) = \frac{\partial}{\partial x}\left(k \frac{\partial T}{\partial x}\right) + \frac{\partial}{\partial y}\left(k \frac{\partial T}{\partial y}\right) + \frac{\partial}{\partial t}(\rho L f_s) \tag{1}
\]

where, \( T \) is temperature, \( x \) and \( y \) are space coordinates along the two faces of the billet caster, \( \rho \) is density, \( k \) is the thermal conductivity, \( C_p \) is the specific heat, \( L \) is the latent heat and \( f_s \) is solid fraction which, considering the non-equilibrium nature of casting solidification (Choudhary and Ganguly, 2007), is computed in the mush using Scheil’s equation:

\[
f_s = 1 - \left( \frac{T - T_w}{T_L - T_w} \right)^{\frac{1}{ke}} \tag{2}
\]

In the above equation, \( T_w \) is the melting temperature of pure iron, \( k_e \) is the partition coefficient and \( T_L \) is the liquidus temperature of steel, which, for carbon composition between 0.5% and 1.0%, is calculated using the following correlation (Choudhary and Ganguly, 2007):

\[
T_L = 1538 - \{44 - 2[\%C] + 52[\%C]^2 + 4.8[\%Mn] + 1[\%Si] + 30[\%P] + 30[\%S] + 1.5[\%Cr] + 4.3[\%Ni] \} \tag{3}
\]

Solidification starts at \( T = T_L \) and is assumed to be completed when the melt temperature reaches the eutectic temperature of the system. The process variables and temperature dependent thermo-physical properties of steel are reported in Table 2 for high carbon steel. Also, electro-magnetic stirring is not considered in the present work. Following expressions are used to calculate enhanced thermal conductivity in the mush (Shibata et al., 2006):

\[
0 \leq f_s \leq 0.3 \quad k_{eff} = \beta k_L \\
0.3 < f_s \leq 0.8 \quad k_{eff} = f_s k_L + (1 - f_s) \beta k_L \\
0.8 < f_s \leq 1.0 \quad k_{eff} = f_s k_L + (1 - f_s) k_L \tag{4}
\]

Since the experiments on billets (Choudhary and Ganguly, 2007) were conducted without electro-magnetic stirring, a value of \( \beta = 2 \) is adopted in this model (Shibata et al., 2006).

Table 2  
Thermo-physical parameters of steel

<table>
<thead>
<tr>
<th>Process variable</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Melt superheat range (K)</td>
<td>9–47</td>
</tr>
<tr>
<td>Liquidus temperature (K)</td>
<td>1,747</td>
</tr>
<tr>
<td>Latent heat of solidification (J kg⁻¹)</td>
<td>271,954</td>
</tr>
<tr>
<td>Specific heat of liquid steel (J kg⁻¹ K⁻¹)</td>
<td>824</td>
</tr>
<tr>
<td>Thermal conductivity of liquid steel (W kg⁻¹ K⁻¹)</td>
<td>34</td>
</tr>
<tr>
<td>Emissivity of steel</td>
<td>0.8</td>
</tr>
<tr>
<td>Density of liquid steel (kg/m³)</td>
<td>7,966–0.619 T</td>
</tr>
<tr>
<td>Density of γ-Fe (kg/m³)</td>
<td>8,218–0.516 T</td>
</tr>
<tr>
<td>Thermal conductivity of γ-Fe (W kg⁻¹ K⁻¹)</td>
<td>21.6–0.00835 T</td>
</tr>
</tbody>
</table>
2.1.2 Initial and boundary conditions

Molten steel coming from tundish is initially assumed to be at a uniform temperature $T_h$. The heat transfer boundary conditions, employed in different zones as the billet solidifies, are described below:

- **Mould zone**: assuming that the heat flux in this region does not vary across the mould width, Savage and Prichard’s expression for heat flux can reliably be used for estimating the total heat transfer.

$$q_m = \left(2.67 - 0.33 \frac{z}{U}\right) \times 10^6 \text{[Wm$^{-2}$]}$$

(5)

where, $z$ is the distance from the meniscus and $U$ is the casting speed. This expression can be easily integrated on the billet surfaces to calculate the total heat flow.

- **Spray zone**: in this region, three primary mechanisms of heat transfer simultaneously operate – forced convective cooling by water jets, conductive cooling through roll contacts and radiative cooling from billet surface. Since the heat extracted from caster surface is predominantly through impinging water sprays, the other two contributions are neglected and the heat equation becomes:

$$q_s = h_s (T_s - T_w)$$

(6)

where, $h_s$ is the spray heat transfer coefficient that depends on the water flow rate, $W$ (in l/m$^2$s) in each nozzle as:

$$h_s = 165.0 W^{0.75}$$

(7)

The spray zone length is sub-divided into three regions for flexibility of cooling: spray ring region (just after the mould), 1A–1B region (after the spray ring) characterised by moderate cooling rate and 2A–2B region (after 1A–1B region) characterised by low cooling rate (Shamsi and Ajmani, 2010). The heat transfer coefficient values in this region are difficult to obtain due to the deposition of a vapour film on the billet surface but have been quite accurately estimated for the CC1 billet caster, Tata Steel, and are summarised in Table 3.

<table>
<thead>
<tr>
<th>Zone</th>
<th>Heat transfer coefficient (Wm$^{-2}$ K$^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>2 m/min</td>
</tr>
<tr>
<td>Spray ring</td>
<td>1,540</td>
</tr>
<tr>
<td>1A–1B</td>
<td>1,060</td>
</tr>
<tr>
<td>2A–2B</td>
<td>660</td>
</tr>
</tbody>
</table>

**Source:** Shamsi and Ajmani (2010)

- **Radiation zone**: the billet surface in this region is subjected to air cooling alone. Considering the convective heat transfer due to air boundary-layer to be significantly less than the radiation heat transfer, the expression for heat flux in this region is given by the Stefan-Boltzmann expression alone:

$$q_r = \sigma \varepsilon_r (T_s^4 - T_w^4)$$

(8)

where, $\sigma$ is the Stefan-Boltzman constant and $\varepsilon_r$ is the emissivity of the surface (Shamsi and Ajmani, 2010).

2.1.3 Simplified CET criterion

Hunt’s critical gradient condition for fully equiaxed growth is given by the following inequality (Hunt, 1984):

$$G < 0.617 (N_0)^{0.3} \left(1 - \frac{\Delta T_N}{T_r} \right)^{0.5}$$

(9)

where, $G$ is the thermal gradient (K/m) at the dendrite tip, $N_0$ is the equiaxed nuclei density (m$^{-3}$) and $\Delta T_N$ and $\Delta T_c$ are the nucleation and constitutional undercoolings respectively at the dendrite tip. $\Delta T_c$ is defined as:

$$\Delta T_c = \left(\frac{RC_0}{A}\right)^{0.5}$$

(10)

$$A = \frac{D}{8m(k-1)\Gamma}$$

(11)

where, $R$ is velocity of columnar front, $D$ is the diffusion coefficient of solute element $C_0$ (wt%) in liquid, $m$ is the liquidus slope, $k$ is the partition coefficient and $\Gamma$ is the Gibbs-Thomson parameter. Taking $C_0$ as the carbon equivalent of the system (Ginzburg and Ballas, 2000) and using data from literature (Mapelli and Baragiola, 2008; Won and Thomas, 2000), the values of different parameters in the above equation are estimated as: $D = 1.83 \times 10^{-5}$ m$^2$s$^{-1}$, $m = -78.0$ K/(wt%), $k = 0.34$ and $\Gamma = 1.9 \times 10^{-7}$ K m. The material constant $A$ for the above set of parameters for high carbon steel comes out to be: $A = 2.34 \times 10^4$ m wt% s$^{-3}$ K$^{-2}$. Also, equation (9) can be further simplified if it is assumed that $\Delta T_N \ll \Delta T_c$.

$$G < 0.617 (N_0)^{0.3} \left(\frac{RC_0}{A}\right)^{0.5}$$

(12)

This assumption was confirmed to be reasonable by Koseki and Inoue (2001) through analysis of the welding zone in ferritic stainless steel. Theoretically, there can be various kinds of substrates present with varying degrees of nucleation efficiency, which can result in a spread of the nucleation undercooling. Such a possibility has previously been investigated by Martorano and Biscuol (2009) who used normal and log-normal distributions of nucleation undercooling. It will, however, require some work before applying this concept to complex casting operations where the source of substrates is difficult to classify.

The parameters $G$ and $R$ are obtained by solving equation (1) iteratively. It is further assumed that the equiaxed grains are spherical and get heterogeneously nucleated on the substrate particles.
2.1.4 Effect of melt superheat on bulk nucleation sites

Nuclei in CC come from various sources, such as heterogeneous nuclei formed on mould walls, inclusions or fragments of dendrites. All these contribute to the parameter \( N_0 \) in equation (12). In most of the studies, \( N_0 \) is either obtained from post solidification analysis or is calibrated to match the experimental observation on CET. It is assumed that for a given mould-casting system which includes alloy composition, cleanliness of the melt, incoatings concentration, etc., a constant \( N_0 \), which provides a reasonable prediction of CET, can be used. These models have been successful in depicting the variation of CET with cooling rate, composition and incoatings’ concentration. However, these models, when employed in their current form, show only a small variation in CET with respect to superheat (Streffelini et al., 2011; Duggan et al., 2015).

On the other hand, it is experimentally well established that CET has strong dependence on initial melt temperature (Choudhary and Ghosh, 1994; Doherty et al., 1977). Studies have shown that chilled crystals near the mould wall which drift towards the centre to form central equiaxed zone, become highly susceptible to remelting which significantly reduces the effective number density of equiaxed grains. Also, as demonstrated through ingot casting experiments on Al-alloys (Chalmers, 1963), the reduction in this number density at higher melt temperatures is sufficient for it to overcome the effects of slower dendritic growth. Therefore, for high melt superheats, this phenomenon becomes prominent and can hardly be ignored. Since there are no accurate analytical expressions available in literature describing this behaviour, an empirical correlation has been used (Chaube et al., 2015):

\[
N_0 = C_1 \exp\left(-C_2 (T_L + \Delta T)\right)
\]  

(13)

where, \( \Delta T \) is the melt superheat and \( C_1 \) and \( C_2 \) are adjustable constants which can be fine-tuned depending on the alloy system and experimental conditions.

2.2 Spot segregation

Considering the non-equilibrium nature of casting solidification, simple analytical models like the Gulliver-Scheil model or Clyne-Kurz model for microsegregation have been used for predicting CLS (Choudhary and Ghosh, 1994; Matsumiya et al., 1984; Tsuchida et al., 1984). However, all these models underestimate or overestimate the extent of solute segregation depending on the value of Fourier number for each of the species (Won and Thomas, 2001).

The formulation used in this work (Won and Thomas, 2001) takes into account the effects of multiple components, parabolic growth dynamics of dendrites and coarsening. This formulation was rigorously validated by the authors through comparison with experimental observations and accurate finite-difference model calculations and is, therefore, reliable. It assumes complete diffusion in liquid phase, local equilibrium at solid-liquid interface and negligible nucleation undercooling and fluid flow effects. The mathematical formulation of the model is expressed as:

\[
C_{L,i} = C_{0,i}\left[1 + f_i (\beta k_i - 1)\right]^{(1-k_i)/(\beta k_i - 1)}
\]  

(14)

where \( C_{L,i} \) is the liquid-concentration of a given solute element at the solid-liquid interface, \( C_{0,i} \) is the initial liquid concentration, \( k_i \) is the equilibrium partition coefficient for that element and \( \beta \) is a back-diffusion parameter that is quantified as:

\[
\beta = 2(x_i + \alpha^C) \left[1 - \exp\left( -\frac{1}{\alpha_i + \alpha^C} \right) \right]
\]  

(15)

\( \alpha^C = 0.1 \) in the above equation is the coarsening parameter and \( \alpha_i \) is the Fourier number for solute element \( i \) given by:

\[
\alpha_i = \frac{D_{s,i} t_f}{X^2}
\]  

(16)

where, \( D_{s,i} \) is the diffusion coefficient of solute element \( i \) in the solid phase, \( t_f \) is the local solidification time and \( X \) is the length scale of the microsegregation domain, usually estimated as half of the secondary dendritic arm spacing (\( \lambda_2 \)).

\[
X = \frac{\lambda_2}{2}
\]  

(17)

Above equations are solved using the numerically obtained \( t_f \) values from solidification model. The formation mechanism of spot like segregations is solidification of trapped liquid spheres in a spherically symmetrical manner from the outer shell to the centre (Tsuchida et al., 1984).

3 Numerical technique

Heat equation is discretised using a finite difference method with an explicit, forward in time, central differencing scheme. A Fortran code is written that evaluates \( G, R \) and \( t_f \) across the billet cross-section as solidification progresses. \( R \), which is the columnar growth velocity is represented by the isotherm velocity for \( f_i = 0.3 \). \( t_f \) represents the local solidification time for nodes and is used for estimating \( \lambda_2 \) and the maximum segregation ratio. Solidification is assumed to be complete when the melt temperature reaches the eutectic temperature of steel.

The simulation domain is a quarter cross-section of billet (62.5 mm × 62.5 mm) and the grid for computation is discretised using 40 × 40 spatial mesh points. This ensures sufficient mesh points to smoothly represent the rapidly changing thermal profile and the discontinuities in heat flux encountered at the boundaries of the phase change region. The explicit finite difference method also has a stability imposed limit on the maximum time-step that can be used. In this case, an initial time-step size of 0.05 s was adopted to ensure stability and smoothness of the solution and was
increased to 0.2 s in the later stages of solidification. The tracking of columnar front is based on the fact that the isotherm velocity is equal to the dendrite-tip velocity at the front. This front-tracking method is easy and efficient to implement and is found to be stable in 2D cases (Wang and Beckermann, 1994). However, complex solidification conditions with melt convection and solid movement require more sophisticated schemes to track the CET boundary.

4 Results and discussions

The solidification model described in Section 2 is applied to high-carbon steel, whose composition is listed in Table 4. Representative 2D simulations were carried out on a quarter section of billet (62.5 mm × 62.5 mm) to simulate real plant conditions (Shamsi and Ajmani, 2010). Equations (1) and (2) were solved using the numerical procedure outlined in Section 3. Figure 3 shows the predicted shell thickness by tracking liquid fraction in the mould region. It was seen that with a grid configuration of 40 × 40 spatial mesh points, the solution was sufficiently stable with only minor fluctuations in shell thickness. Further refining the mesh (to 50 × 50 nodes) did not significantly change the shell thickness profile and the solution was grid-independent. Therefore, 1,600 mesh points have been used for calculations. The predictions show a good qualitative match with the observed shell thickness profiles of low-carbon steel billets for CC1 caster of Tata Steel (Shamsi and Ajmani, 2010). The shell thickness at the exit of the mould is around 7 mm. The fact that the predicted values in this case are relatively lower can be attributed to wider solidification range of high-carbon steel considered in the present study. In Figure 4, the contour plots of temperature across the modelling domain, i.e., quarter cross-section of billet, are shown for four different positions. It can be seen that the temperature at the centre close to the cut-off point (~16 m) is around 1,650 K which is less than the solidus temperature of steel for the given composition. This means that complete solidification takes place before the cut-off point. Figure 5 represents the simulation results for G and R corresponding to \( f_s = 0.3 \). In the columnar region, parameters R and G decrease with increasing distance from the centre of billet surface. In the central region, however, R increases owing to a higher dendritic growth rate in the final stages of solidification. This behaviour was observed by Long et al. (2010) and Mapelli and Baragiola (2008) too. The time for complete solidification of billet is estimated to be around 283 s, for which, the metallurgical length comes out to be around 11.8 m.

4.1 Morphological predictions and model validation

The morphological selection map for given input parameters and process variables is represented in Figure 6. The increase in slope of log (G) versus log (R) plot at higher G values is consistent with experimental observations on boron grade steel with similar composition (Mapelli and Baragiola, 2008).

Table 4 Melt chemistry of steel under investigation

<table>
<thead>
<tr>
<th>% C</th>
<th>% Mn</th>
<th>% Si</th>
<th>% P</th>
<th>% S</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.75</td>
<td>0.66</td>
<td>0.16</td>
<td>0.02</td>
<td>0.02</td>
</tr>
</tbody>
</table>

Source: Choudhary and Ganguly (2007)
Figure 4  Temperature contours (in K) across the modelling domain – quarter cross-section of billet – after exit from, (a) mould region (b) 1A–1B region (c) 2A–2B region (d) spray zone for a casting speed of 2.5 m/min and a superheat of 21 K (see online version for colours)

Figure 5  Calculated solidification parameters along the mid-plane of billet surface
4.1.1 Effect of melt superheat on CET

To validate the model and study the influence of initial melt temperature on CET, 2D simulations were carried out for four values of tundish superheat (9 K, 21 K, 33 K, 47 K) and a casting speed of 2.5 m/min as in the experiments (Choudhary and Ganguly, 2007). The values of constants in Equation 13 for this study are $C_1 = 3.113 \times 10^{27}$ and $C_2 = 0.0267$. Equiaxed zone boundary is marked in Figure 7(a) for each of the above superheats. It is seen that for a low tundish superheat of 9 K, the location for onset of CET is very close to the billet surface and there is a predominantly equiaxed structure. Figure 7(b) shows a comparison between the predicted and measured equiaxed area-fraction values for the 9–47 K superheat range. The values have been plotted with and without Equation 13 to demonstrate the influence of $N_0$ in the model. A reference value of $N_0 = 10^7$ m$^{-3}$ is taken for a superheat of 21 K (Chaube et al., 2015). It is evident that the model predictions, without the proposed empirical relation, grossly underestimate the effect of superheat on CET. When the superheat is increased from 9 K to 47 K, the number density of equiaxed nuclei reduces by ~65% which drastically suppresses equiaxed growth. The variations in $G$ and $R$ alone, however, are too insignificant to produce any major variations in CET. A similar study on steel billets reported a weak variation of CET with $\Delta T$ (Straffelini et al., 2011) by assuming constant $N_0$, which is not in agreement with the observed experimental trends.

4.1.2 Effect of casting speed on CET

Casting speed directly affects the evolution of solidified shell along caster length. Lower casting speed results in a thicker and stronger solidified shell at mould exit which reduces bulging and severity of CLS. However, it is a direct measure of productivity and cannot be compromised below a certain limit.

To quantify the influence of casting speed on morphology and the metallurgical length, representative simulations were run for three casting speeds: 2 m/min, 2.5 m/min and 3 m/min, using the CET model validated above. During plant operations, changes in casting speed are always accompanied with adjustments in the secondary cooling intensity through spray nozzles (Table 3) (Shamsi and Ajmani, 2010). Figure 8 depicts the boundary of fully-equiaxed zone for the considered range of casting speeds. For a change in the casting speed from 2 m/min to 3 m/min, there is almost a 50% reduction in the equiaxed zone area. This is because faster cooling promotes increased thermal gradients, and hence, unfavourable conditions for equiaxed grain growth. Also, the metallurgical length and total solidification time are increased (Table 5) due to shortened holding time of billet in the secondary cooling zones. Strictly speaking, there should be some change in the equiaxed crystal density with a change in the casting speed as well. However, in the considered range of casting speeds, this variation is hardly pronounced and is ignored (Zeng and Chen, 2010). The casting speed was further increased beyond 3 m/min and simulations were run using the extrapolated heat transfer coefficient values from Table 3. It was seen that for a casting speed of 3.3 m/min, the metallurgical length became almost equal to 16 m, i.e., the caster cut-off length. It is, therefore, the theoretical limit of casting speed for given carbon composition and processing conditions. This is in contrast to ~4 m/min limit estimated for the same billet caster, but for low-carbon steel. The wide freezing range of high-carbon steel in this case increases the solidification time and hence, lowers the cut-off for maximum casting speed.
Table 5  Influence of casting speed on solidification parameters

<table>
<thead>
<tr>
<th>Casting speed (m/min)</th>
<th>CET (from surface) (mm)</th>
<th>Area fraction of equiaxed zone</th>
<th>Metallurgical length (m)</th>
<th>Solidification time (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>47.5</td>
<td>0.56</td>
<td>9.27</td>
<td>278</td>
</tr>
<tr>
<td>2.5</td>
<td>39.8</td>
<td>0.38</td>
<td>11.79</td>
<td>283</td>
</tr>
<tr>
<td>3</td>
<td>33.4</td>
<td>0.28</td>
<td>14.32</td>
<td>286</td>
</tr>
</tbody>
</table>

Figure 7  CET as a function of melt superheat, (a) transition location for four different superheats (b) model validation – comparison with experiments
4.1.3 Secondary dendritic-arm spacing (SDAS)

SDAS is an important characterisation parameter of the solidification microstructure. On the basis of local solidification time $t_f$, the evolution of SDAS ($\lambda_2$) can be tracked along the billet mid-plane using following correlation:

$$\lambda_2 = M'(t_f)^{1/3}$$  (18)

where $M'$ is a material constant, the expression for which has been derived (Mapelli and Baragiola, 2008) considering the role of three most important alloying elements. The calculated value of $M'$ for the considered alloy system is around $5.39 \times 10^{-5}$. Figure 9 shows the variation of SDAS as a function of distance from the billet surface. In the chill zone, very close to the billet surface, the computed SDAS is small (~25 μm) which increases to around 170 μm near the boundary of equiaxed zone. This increase is consistent with the observed SDAS variation in the columnar region (Choudhary and Ganguly, 2007) and is due to reduced cooling at the exterior surfaces of the billet. The dip in the experimental values near the centre, however, can be attributed to carbon enrichment and changed mobility of dendrites and cannot be captured using equation (18). Also, there could be instability or non-uniformity in heat extraction from the billet surfaces during real casting.
4.2 Segregation predictions

In this study, Equation 14 is employed for obtaining liquid concentration profiles as a function of \( f_s \) using the diffusivity data available in literature for C, S and Mn. A value of \( t_f = 283 \) s (casting speed = 2.5 m/min) computed from the solidification model is used to estimate the Fourier numbers from equation (16). Table 6 shows the diffusivities of the solute species in \( \gamma \) phase, their Fourier numbers and the back-diffusion parameters. As already established (Stefanescu, 2015), for higher values of \( \alpha \), the Brody-Flemings equation predicts less enrichment in the liquid phase than does the Lever rule and is physically unreasonable. The Clyne-Kurz model too, in its original form, slightly under predicts microsegregation for very low \( \alpha \) values while the Thomas and Won’s model used in the present analysis is accurate for a wide \( \alpha \) range. Figure 10 shows the variation of liquid composition with fraction of solid in a small solidifying drop of 1 mm diameter at the centre. This size is of the order of experimentally observed width of segregation spots (Choudhary and Ganguly, 2007). Diffusion through the closer-packed austenite structure is slow, which enhances microsegregation and depresses the solidus temperature significantly below equilibrium. The model predicts high enrichment of S in the liquid phase, which is consistent with its very small partition coefficient value in \( \gamma \) phase. In principle, the specie concentration, shape and size of the originally trapped liquid steel should be carefully determined based on the solidification morphology and flow effects during later stages of solidification. However, in this study, the initial composition of the enriched liquid drop \( C_{(\text{drop})} \), is assumed to be equal to the concentration of liquid steel among dendrites with \( f_s = 0.99 \) calculated using equation (14), similar to the assumption made by Matsumiya et al. (1984). Also, considering the spherically symmetric manner of solidification, the total fraction of solid at any instant in the drop is approximated as the ratio of the volume of solidified shell to that of the liquid drop (Tsuchida et al., 1984). With this assumption, equation (14) can be rewritten as:

\[
C_{s,i} = k_i C_{(\text{drop})} \left( R/R_0 \right)^3 + \beta_i k_i \left( 1 - \left( R/R_0 \right)^3 \right) \left( 1 - k_i/(\beta_i - 1) \right) \tag{19}
\]

where, \( R_0 \) is the initial radius of solidifying drop and \( R \) is the radius of liquid sphere remaining at any given instant. Figure 11 depicts the segregation ratios in the solid phase of the three species as a function of distance from the centre of drop after solidification is complete. The maximum segregation ratio for all three species, \( (C_{(i)}/C_{(0)})_{\text{max}} \), is clearly achieved at the centre and is given in Table 7. The calculated values show a close match with the reported experimental findings of Choudhary and Ganguly (2007) which validates the model to some extent. A more sophisticated modelling framework of segregation, however, requires studying flow-driven macrosegregation at the grain-size scale and will be considered in future investigations.

<table>
<thead>
<tr>
<th>Specie</th>
<th>( D^i ) ( (m^2/s) )</th>
<th>( \alpha_i )</th>
<th>( \beta_i )</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>( 1.056 \times 10^{-11} )</td>
<td>0.131</td>
<td>0.479</td>
</tr>
<tr>
<td>S</td>
<td>( 4.467 \times 10^{-12} )</td>
<td>0.056</td>
<td>0.397</td>
</tr>
<tr>
<td>Mn</td>
<td>( 2.727 \times 10^{-15} )</td>
<td>0.000034</td>
<td>0.315</td>
</tr>
</tbody>
</table>

Source: Matsumiya et al. (1984)

Figure 10  Species’ concentrations in the liquid phase predicted using a simple microsegregation model of Won and Thomas (see online version for colours)
Table 7  Chemistry of the solidifying drop

<table>
<thead>
<tr>
<th>Specie</th>
<th>$C_{h,\text{drop}}$</th>
<th>$(C_i/C_{h,\text{drop}})_{\text{max}}$</th>
<th>$(C_i/C_i)_{\text{min}}$</th>
<th>$(C_i/C_i)_{\text{max}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>0.995 (wt %)</td>
<td>1.37</td>
<td>1.72</td>
<td>1.9</td>
</tr>
<tr>
<td>S</td>
<td>0.0268 (wt %)</td>
<td>2.24</td>
<td>3.00</td>
<td>2.64</td>
</tr>
<tr>
<td>Mn</td>
<td>0.768 (wt %)</td>
<td>1.17</td>
<td>1.29</td>
<td>1.25</td>
</tr>
</tbody>
</table>

Figure 11  Radial concentration profile of species in the solidified drop (see online version for colours)

5 Conclusions

A two-dimensional heat transfer and solidification model has been developed and validated for simulating the morphology and spot-segregation characteristics of CC billet and obtaining useful quantitative predictions related to the casting process. Based on the study, following major conclusions are drawn:

1  Parametric studies show that increasing the casting speed or melt superheat significantly reduces the equiaxed zone area and increases the metallurgical length, both of which can negatively impact the mechanical properties of finished products. This is in line with the experimental observations on CET.

2  An empirical correlation, depicting the variation of equiaxed nuclei density with melt superheat is incorporated in the solidification model. With this equation, model results show a reduction in the equiaxed zone area by ~73% as the superheat is increased from 9 K to 47 K. This agrees fairly well with the experimentally measured reduction in area for the considered superheat increase and therefore, correctly depicts the industrial trend.

3  An attempt has been made to analyse small semimacrosegregation spots during CC for three species – C, S and Mn – using a simple microsegregation model proposed by Thomas and Won. This model can be reliably used regardless of the value of solute’s back-diffusion coefficient in solid.

4  Maximum segregation values for C, S and Mn as calculated from the above microsegregation model are 1.72, 3.00 and 1.29 respectively. This shows good consistency with the experimentally observed peak segregation ratios of 1.9, 2.64 and 1.25 for high-carbon steel billets.

References


