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Online Modelling of Heat Transfer, Solidification and Microstructure in Continuous Casting of Steel

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Abstract. Advanced numerical simulation models for continuous casting of steel were developed in Finland by Casim Consulting and Aalto University in cooperation with the University of Oulu and the steel industry. The aim was to develop models that are scientifically rigorous, but also computationally fast enough to be used in online applications. The models developed are a transient three-dimensional heat transfer model, CastManager, and a solidification and microstructure model, IDS. The computing time of these models are short, and they are integrated together in one online concept. This concept is installed in the automation systems of four slab casters in Finland. Testing and validation work is in progress. The system simulates the important heat transfer, solidification and microstructural phenomena in continuous casting online. The future aim is that this information will be used for online quality control and for optimizing the process conditions to avoid formation of defects. Many quality indices have already been developed. A steady state version of the CastManager tool has also been developed, called Tempsimu.

1. Introduction

Computational simulation and modelling of different phenomena in casting have greatly helped to solve practical problems in industrial casters and to improve process practices and control. Altogether, a deeper understanding of the complex solidification phenomena and transformations of the microstructure is still needed to respond to increasing requirements. For this purpose, advanced numerical simulation models for continuous steel casting were developed in Finland by Casim Consulting and Aalto University in cooperation with the University of Oulu and the steel industry. The aim was also to develop models that are scientifically ambitious but also to make these models computationally fast enough to be used in online applications of process control and quality prediction. In online applications, fast computing is of special importance. During the years, many kinds of models for continuous casting have been introduced in international journals, such as models for heat transfer and microstructural phenomena. The published microstructural models are often based on concepts,

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which are so time consuming that they cannot be applied in online applications. Typical concepts of this kind are cellular automata and phase field methods. Fast computing is also important for online heat transfer models because it allows a more detailed determination of the boundary conditions, leading, thus, to more accurate and realistic results.

The models developed and presented in this paper are a transient three-dimensional heat transfer model, CastManager [1], and a solidification and microstructure model, IDS [1–3]. The computing time of these models are short, and they are now integrated together in one online concept. The system simulates the important phenomena in continuous casting online. The future aim is to use this information for online quality control and for optimizing the process conditions to avoid defect formations. Many quality indices have already been developed. A steady state version of the CastManager tool has also been developed, called Tempsimu. This paper presents the developed models and the integrated on-line concept with some case examples.

2. CastManager and Tempsimu heat transfer models

CastManager and Tempsimu are heat transfer modelling software for continuous steel casting. They calculate strand temperatures, mold temperatures and temperature-related data (such as the shell thickness and total mold heat flux) as a function of the following main data:

- secondary cooling components: rolls, nozzles and radiation zones,
- steel grade (thermophysical material properties),
- strand geometry, mold geometry, mold material properties including the possibility to have different material layers (e.g. coating layers),
- casting variables: casting speed, superheat, spray cooling water flow rates.

CastManager is a software for transient online applications, while Tempsimu is a software for steady-state modelling. Tempsimu can be applied for instance to analyze the existing secondary cooling system and to study new alternatives (spray and roll configurations, cooling water flow rates). The programs consist of two separate modules: a three-dimensional mold model and a three-dimensional strand model. They are run iteratively, and the so-called gap heat transfer coefficient, which is a function of the strand temperature, is used to link them. In the calculations, the Leidenfrost effect and the effect of melt convection (fluid flow) are taken into account. Material data is calculated with the InterDendritic Solidification (IDS) package, which directly gives the data file needed. In many heat transfer models, a fixed grid is used. Our tools also use the fixed grid approach. To take the shrinkage and the mass balance into account, CastManager and Tempsimu use constant density. It is important to take care that the mass inlet is equal to the mass outlet in the casting model. To do this, we define the grid horizontal dimensions to be the dimensions of the mold at the meniscus level and, for the density, we give its value at the solidus temperature. With the latter treatment, we take into account the solidification shrinkage taking place during solidification.

The fluid flow, heat transfer, and solidification processes in continuous casting are interlinked and therefore, for a complete heat transfer model, a fully linked approach is needed. These kinds of linked models have been published in the literature and typically they have been made using a commercial CFD tool. Their use is very time consuming and needs a professional user. In addition, the calculation times are very long, and the models cannot be used online. A simplified approach uses the so called effective thermal conductive concept, in which the effective thermal conductivity takes into account the effects of fluid turbulence and convection on heat transfer. It is widely agreed that this approach gives reasonable results. An additional benefit is that the models based on this concept are very fast. CastManager and Tempsimu use the effective thermal conductive concept.

In CastManager, heat transfer and solidification in the strand are defined by equation (1), which can be described according to equation (2) when the enthalpy and Kirchhoff's transformations are applied; they are described by equations (3) and (4), respectively.

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$$\rho c \frac{\partial T}{\partial t} + \frac{\partial v \rho c T}{\partial z} = \frac{\partial \left(k_{\text{eff}} \frac{\partial T}{\partial x}\right)}{\partial x} + \frac{\partial \left(k_{\text{eff}} \frac{\partial T}{\partial y}\right)}{\partial y} + \frac{\partial \left(k_{\text{eff}} \frac{\partial T}{\partial z}\right)}{\partial z} + Q, \tag{1}$$

$$\frac{\partial H}{\partial t} + v \frac{\partial H}{\partial z} = \Delta K(T), \tag{2}$$

$$H(T) = \rho \int_0^T c(\xi)\, \mathrm{d}\xi + \rho L\big(1 - f_{\text{s}}(T)\big), \tag{3}$$

$$K(T) = \int_0^T k_{\text{eff}}(\xi)\, \mathrm{d}\xi, \tag{4}$$

where $H(T)$ is the enthalpy function, $K(T)$ is the Kirchhoff's function, t is time, k_{eff} is the effective thermal conductivity, c is the specific heat capacity, L is latent heat, f_{s} is the solid fraction, T (and ξ) is the temperature, ρ is the density and v is the actual casting speed in the casting direction. The enthalpy function H includes the effect of all phase transformations. Equation (5) describes the mold model where all variables are the same as in the strand model except that there are no phase transformations, so $L = 0$. In a numerical solution, the strand and mold models are iterated together so far that convergence is reached. In Tempsimu, the transient terms are not needed.

$$\frac{\partial H(T)}{\partial t} = \Delta K(T). \tag{5}$$

The boundary condition between the strand and the mold in the strand model is defined as:

$$-\nabla K(T) \cdot \vec{n} = h_{\text{gap}}(T - T_{\text{ext}}), \tag{6}$$

where $\vec{n}$ is the unit vector of outward normal to boundary of the strand, h_{gap} is the gap heat transfer coefficient, T is the strand surface temperature and T_{ext} is the external temperature, in this case the temperature of the mold surface. The gap heat transfer coefficient is a function of the strand surface temperature, but it also depends on the steel grade and the type of the mold powder. Equation (6) is also used as the boundary condition for the hotter side of the mold model, where h_{gap} is the same gap heat transfer coefficient as for the strand model, but T_{ext} is now the temperature of the strand surface, which is calculated by the strand model. For the colder side, a similar equation is used, but T_{ext} is the temperature of the cooling water and h is a constant. In the secondary cooling zone, the strand model has been divided into calculation domains between a pair of support rolls. This domain has been divided into four different cooling areas that are: the roller contact area, pre-nozzle area, spraying area, after spray and pool water area (post-nozzle area). The boundary equation for these areas is defined as:

$$-\Delta K(T) = h(T - T_{\text{ext}}) + \varepsilon\sigma\big(T^4 - T_{\text{air}}^4\big), \tag{7}$$

where h is heat transfer coefficient, T_{ext} is external temperature, T_{air} is the external temperature for the radiation term, ε is the emissivity value of strand surface and σ is the Stefan–Bolzmann constant. Heat transfer coefficients are defined with specific data and equations and these depend on the type of the roll or spray nozzle, amount of spray water, surface temperature. Accurate boundary conditions form the basis of good predictive capability. Laboratory trials, plant measurements and published data can be used for definitions. The model equations are discretized using fully implicit three-dimensional finite difference (FDM) and upwind schemes. An implicit Crank–Nicholson method is used for time discretization. The resulting algebraic equations are solved using a parallel Gauss–Seidel–Newton–Raphson method.

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3. IDS tool

IDS is a thermodynamic-kinetic-empirical software package, which simulates solidification and cooling related microstructural phenomena, such as solute micro segregation, phase transformations, inclusion and precipitate formation, grain growth and austenite decomposition. IDS can be applied from the liquid state to the as-cast room temperature state and during the reheating treatments of a reheating furnace. The cooling rate can vary during cooling and reheating. The calculation times are very short making the tool suitable for online applications.

The present elements available in IDS are C, Si, Mn, P, S, Cr, Ni, Mo, Al, Cu, N, Nb, Ti, V, Ca, B, O, Ce, Mg and H. IDS consists of several modules and not all elements are included in all modules. As input, IDS requires the nominal steel composition and cooling-heating rates. IDS includes default equations for calculating the dendrite arm spacing and the austenite grain size, as a function of the composition and cooling rate, but the user can use own values too. The simulation of austenite decomposition is based on empirical Continuous Cooling Transformation (CCT) diagrams. The phases considered by IDS are δ-ferrite, α-ferrite, eutectic ferrite, austenite, cementite, pearlite, bainite, α-martensite (bct structure) and ε-martensite (hcp structure).

IDS applies thermodynamic and kinetic theories assuming thermodynamic equilibrium at the phase interfaces. During the austenite to proeutectoid ferrite or cementite transformation, the thermodynamic para-equilibrium condition is assumed, indicating diffusion only for the interstitial elements (e.g. B, C and N). In the austenite decomposition module, phase transformations are mainly based on regression equations optimized from empirical CCT diagrams. The considered elements of this module are C, Mn, Si, Cr, Ni, Mo and B, though Al and Cu will soon be added to the simulation. The user can define whether the nominal composition or the grain boundary dissolved composition is used in the calculations.

The formation and growth of various inclusions from the liquid is based on thermodynamic equilibrium calculations. For precipitates, forming below the solidus temperature, the calculation concept is more complicated, because kinetic phenomena and additional energies, like that of misfit must also be taken into account. For the austenite grain growth, an empirical formula is used. In this formula, the grain growth is reduced by high cooling or heating rates (lack of time), low temperature, and formation of ferrite and precipitates.

IDS also includes a module for the calculation of material properties, such as enthalpy, thermal conductivity and density, as a function of steel composition and cooling rate. More information about the IDS tool, including its databases and additional modules, are available in Refs. [1-3].

4. Integrated system IDS and CastManager/Tempsimu

The IDS tool has been coupled with CastManager for online applications and with Tempsimu to study offline steady state situations. The IDS and CastManager integrated system has been implemented for four slab casters in Finland. Testing and validation work is now in progress. The start and the end of casting, as well as the ladle change, the steel grade change and the width change are also included in the system. The system simulates heat transfer, solidification and microstructural phenomena in continuous casting and the aim is to use it for quality prediction and for optimizing the casting conditions. First, IDS calculates the material data of the steel for CastManager, using the online measured steel composition of the ladle. Then, during the casting process, CastManager gives temperatures and cooling rates to IDS, which calculates the microstructural phenomena and the quality (Figure 1). For describing the strand quality, several quality indices have already been developed. Their testing and validation is in progress. One way to speed up the system calculations is to use a graphics processing unit (GPU) instead of a central processing unit (CPU). This work is also in progress. Similar work has been carried out for the developed reheating system. Correspondingly, this system is called the IDS and FurnaceManager integrated system. It has been installed for one reheating furnace in Finland. Using a GPU for that system was found to accelerate simulations by a factor of 5–13 compared to simulations using the CPU.

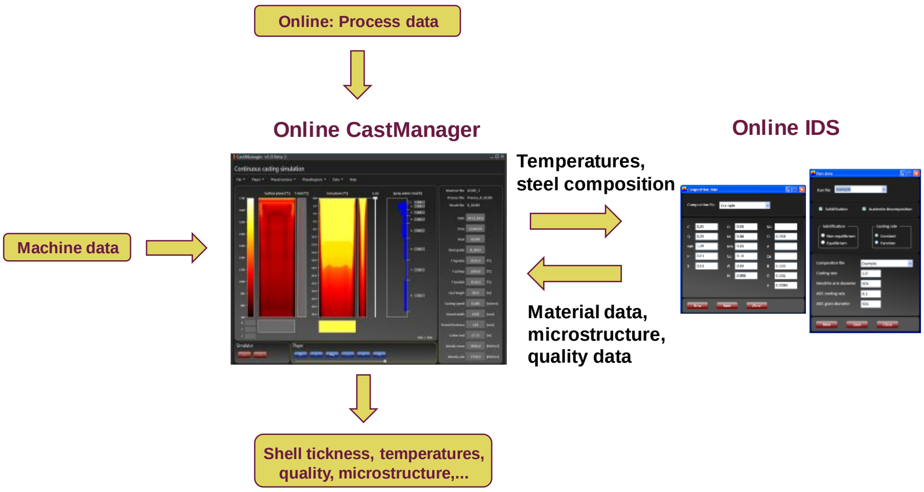

Figure 1. IDS and CastManager integrated online system for continuous casting.

5. Case examples: Quality criteria and grain growth

IDS simulates many microstructural phenomena as a function of the steel composition and cooling/heating rates. From this information, combined with the results of CastManager, several quality indices can be derived. Figure 2 shows two quality criteria (QI_{she} and QI_{str}) as function of carbon content.

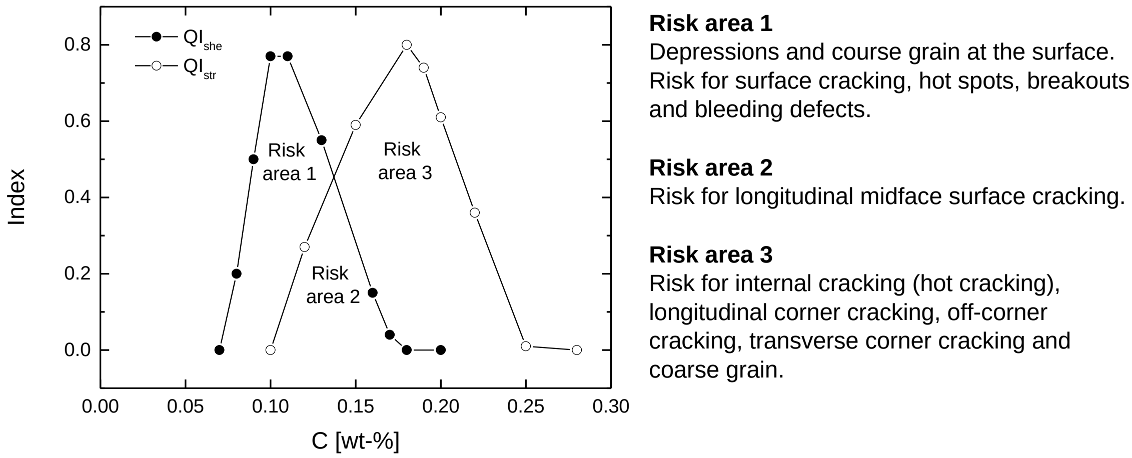

Figure 2. IDS quality criterion values of QI_{she} and QI_{str} for a certain steel composition with increasing carbon content. For stainless steels, these criteria overlap more. High index means high risk for defects.

The QI_{she} is the fraction of delta ferrite at the solidus, minus the fraction at T_{sol}–30 °C. It is known that ferrite to austenite transformation starting just below the solidus causes many problems, because of the shrinkage in this phase transformation. High values of QI_{she} indicate high risks of several types of surface defects, such as hot spots, surface cracking, bleeding, breakout, etc. Typically, problems occur between 0.08 and 0.15 wt-% C in carbon steels, but the alloying and tramp elements tend to change the carbon range. For stainless steels, the highest risk is when the Cr/Ni-equivalent ratio is about two. QI_{str} is the fraction of delta ferrite at T_{ZST} (zero strength temperature, related to the solid fraction of 0.8) minus that fraction at the solidus. If austenite starts to form (from liquid and ferrite) between solid fractions of about 0.8 and 1, the shrinkage of this phase transformation can cause stresses above the solidus, increasing the risk for surface and internal cracks.

The QI_{sol} criterion describes the reduced hot ductility (around the solidus) because of the strong enrichment of S, P and B in the interdendritic liquid, increasing the risk for internal hot cracking. The

QI_{duc} criterion describes the effects of precipitates in reducing the ductility in the low ductility areas of II and III due to the grain boundary sliding (area 2) or the deformation induced proeutectoid ferrite/cementite present at the grain boundaries (area 3). These all increase the risk of transverse corner cracks. Particularly, if QI_{str} and QI_{duc} both have a high value, the risk of transverse corner cracking becomes very high. In that case, the secondary cooling needs to be controlled so that during the bending and unbending processes, the slab corner temperatures remain outside the temperature region of the low ductility area. It is also possible to fine-tune the steel composition, already in the ladle, to pass the highest criteria peaks and thus, to reduce the risk of defects. Many other quality criteria are also under work.

Figure 3 shows an example of the austenite grain growth in carbon steel with different carbon contents. The growth is restrained by the grain boundary ferrite and the Nb(C,N) precipitation. Carbon has clear effects on both of these phenomena. Note that in the 0.05 wt-% C steel, the grain growth starts over 50 °C below the solidus, because of the high ferrite content present. Its final grain size however, is highest, due to the low amount of Nb(C,N), which is not capable of restraining the grain growth so effectively.

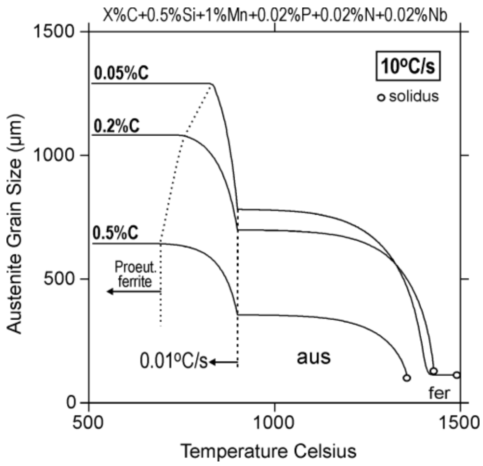

Figure 3. Calculated austenite grain growth in three low-alloyed steels containing 0.05 wt-% C, 0.2 wt-% C and 0.5 wt-% C, cooled with a rate 10 °C/s above 900 °C and with 0.01 °C/s below 900 °C.

6. Conclusions

Numerical simulation models for continuous casting of steel have been developed in Finland by Casim Consulting and Aalto University in cooperation with the University of Oulu and the steel industry. These models are intended to provide a detailed description of the main phenomena, while being sufficiently fast for online use. The main tools developed are the CastManager and Tempsimu heat transfer models and the IDS package, which can be coupled for a given task or online concept. The potential of the model was illustrated with predictions for quality criteria and grain growth.

Acknowledgements

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