- Abziehen der festen Strangschale mit der Gießgeschwindigkeit
- Bewegung der Strangschale entsprechend den Druckverhältnissen (Implementierung verschiedener Materialmodelle)
- Kopplung von Stahl und Schlacke im flüssigen Bereich über die Oberflächenspannung
- Ausbildung eines Gießschlackenwulstes an der Kokille im Bereich des Übergangs von festem auf flüssiges Gießpulver
- Zuordnung anderer Stoffgrößen zu allen Bereichen
- Oszillation der Kokille (Hub, Frequenz, Form) als beliebige Funktion der Zeit
- Variationsmöglichkeiten aller geometrischen Größen

Mit dem Modell werden untersucht:

- Ausbildung und Entstehung der Hubmarken (Form, Tiefe, ...)
- Einfluss der Stoffgrößen (Stahl- und Gießpulvereigenschaften)
- Gießpulververbrauch
- Trends bei Variation der Gießparameter wie Hub, Frequenz und Oszillationsform

Das Modell wurde im Frühsommer 2001 fertig gestellt und wird derzeit getestet. Eine Auswertung der Ergebnisse (Abb. 8), Gegenüberstellungen mit gemessenen Daten und Diskussion führen, wie bei jeder Computermodellierung eines Prozesses, zu einem tieferen Verständnis der physikalischen Vorgänge. Auf diese Erkenntnisse aufbauend werden Betriebsparameter entsprechend angepasst. Dies erhöht die Fertigungssicherheit und gewährleistet eine konstante Qualität des Produktes.

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Simulation of Solidification and Microstructure in Continuous Casting of Steel

C. Bernhard, B. G. Thomas, G. Xia, and C. Chimani

State-of-the-art in modelling of continuous casting of steel – Numerical treatment of solidification problems – Microstructural evolution during solidification – Defect formation in continuous casting – Thermal stress analysis for understanding defect formation – Effect of microstructure – Synthesis of numerical and physical simulation

Simulation von Erstarrung und Mikrostruktur beim Stranggießen von Stahl. Stand der numerischen Simulation des Stranggießens – Numerische Behandlung von Erstarrungsproblemen – Ausbildung der Mikrostruktur – Fehlerbildung beim Stranggießen – Thermo-mechanische Analyse zum Verständnis der Fehlerbildung – Einfluss der Mikrostruktur – Synthese von numerischer und physikalischer Simulation

1. Introduction

The role of numerical modelling in the further improvement of the continuous casting technology will become more and more important, due to the rapid development of hardware and numerical methods. In many previous advances modelling already played a key role, often involving relatively simple calculations for lack of computer performance. Modelling pioneers who contributed to continuous casting understanding include J. K. Brimacombe, I. V. Samarasekera, K. Schwerdtfeger, K. Wuennenberg, H. Fredrikson, T. Emi and many others.

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As voluminous literature exists on computational modelling of solidification technology, it is impossible to give a comprehensive overview due to space limitations. This paper will present a brief survey of the state-of-the-art of numerical modelling of the conventional continuous

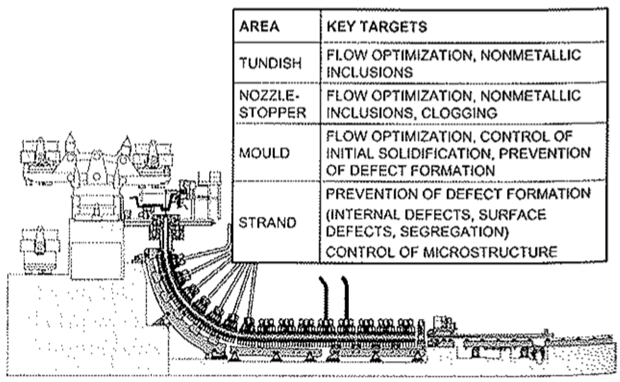


Fig. 1. Schematic of a continuous casting machine with key targets for numerical modelling

casting of steel and a few examples will be taken from the work of the authors in order to illustrate the great variety of targets and methods.

Figure 1 shows a schematic view of a continuous casting machine. The conventional continuous casting process can be characterized by a stationary, oscillating mould. In most cases the liquid steel is fed to the mould from a tundish through a submerged entry nozzle. The tundish serves as buffer between the ladle and the mould, enabling sequence casting and leading to a further homogenization of the melt. The separation of non-metallic inclusions is another important function.

The mould consists of water cooled copper plates or a copper tube. Friction and heat transfer between steel and copper mould are controlled by a thin mould flux layer. The use of oil as lubricant in billet casting becomes less and less common. Initial solidification has a dominating influence on the surface quality of the cast product. The optimization of the conditions for initial solidification in the mould (e.g. mould flux, oscillating mode, liquid flow pattern) is a key target in process and quality control.

At the bottom of the mould, the strand is withdrawn surrounded only with a thin solidified shell. Strand guiding and the cooling of the strand by spray water or air/mist below the mould, the so-called secondary cooling, is another important factor for product quality. Because of its comparably low thermal conductivity, the solidifying steel shell controls heat transfer leading to a protracted distance between the liquid steel level in the mould and the point of solidification of the last residual liquid (metallurgical length). Dependent on casting section (billet, bloom, slab) and casting speed, the metallurgical length extends up to 40 m.

These dimensions, together with the effects of alloying elements (segregation, precipitation), the phase transformation of steels during and after solidification (shrinkage, porosities), or the deformation of the solidifying shell (bulging, unbending), make the continuous casting process a challenging task to control and optimize. Due to the complexity of the process, numerical simulation becomes a major tool for continuous casting engineers, providing a more complete understanding on the entire process.

2. State-of-the-Art in Numerical Modelling of Continuous Casting

The comprehensive numerical simulation of the continuous casting process demands a simultaneous analysis of multi-physics and multi-scale aspects[1]. The modelling of at least the following continuum phenomena is required:
- fluid flow
- heat transfer
- phase changes
- solid mechanics
- electromagnetics
- and their interactions

The computational modelling of such interacting phenomena, by e.g. Finite Element (FE) or Finite Volume (FV) methods is still a challenge, in spite of the rapid development of hardware and numerical methods.

In addition, the physical phenomena are active at various length scales in space and time. For instance, the grain structure of semis will depend on the heat diffusion at the macroscopic scale of the casting, on the solute diffusion at the scale of a grain and of the tip of the dendrite, as well as the atomic adsorption near an embryo during the nucleation. It is thus needed to couple these different length scales and to make the necessary simplifications for the design of a model which is realistic and usable from the viewpoint of limitation in computation time. This coupling is illustrated in Fig. 2. The heat diffusion (as well as the heat exchanges between strand and mould, respectively spray cooling water) should be considered at the scale of the casting. This can be treated with conventional numerical methods, such as Finite Elements or Finite Volume. On the other hand, growth kinetics are dictated by local phenomena around the dendrite tip, at a scale of a few microns. At an intermediate level, the description at the scale of the grains should be made according to "microscopic" models[2].

Mathematical models have been applied to many different aspects of the continuous casting process. Unfortunately, attempts to summarize this work are rare (e.g.[13, 14]), and thus, a comprehensive overview would result in the enumeration of hundreds of papers published during the last decades. From the latest publications, the following trends in numerical modelling of the continuous casting process can be observed:

- *Modelling of fluid flow in the tundish and mould by Computational Fluid Dynamics(CFD)*: mixing models[15], control of steel cleanness in the tundish[16], prevention from clogging and air aspiration[17], fluid flow in the nozzle[18], fluid flow in the mould[19]. CFD combined with water models has become a powerful tool in the optimization of the flow pattern in tundish, nozzle and mould. Many publications focus on fluid flow in the mould and nozzle optimization.
- *Modelling of the initial solidification in the mould*: heat flow[20, 21], mechanical behaviour of the solidifying shell[22], thermal distortion of the mould[23], oscillation mark formation[24], initial shell strength[29]. Most previous heat flow studies focus on shell growth and temperature in the spray zones. There are only a few studies on initial solidification, the formation of surface defects in the mould and friction between strand and mould.
- *Thermo-mechanical modelling of deformation related defects*: bulging[25, 26], straightening[27], micro-mechanical modelling of ductility minima[28].

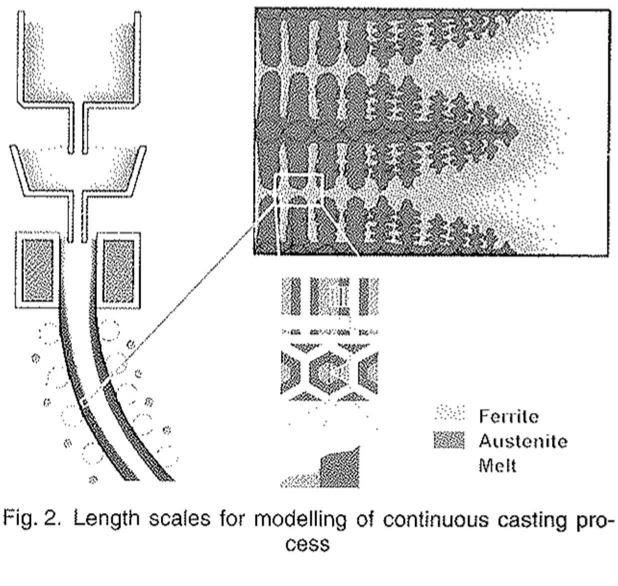


Fig. 2. Length scales for modelling of continuous casting process

Besides these publications on mathematical modelling, numerous work on physical models, experiments and measurements on operating casters has been done, necessary for the validation of the mathematical models.

2.1 Flow Simulation

Fluid flow is associated with many of the most important quality problems in the continuous casting process, Fig. 3. Because it is the last liquid processing step, poor control of flow in the mould can cause many defects that cannot be corrected. Problem sources in the mould include: air entrainment due to inadequate surface coverage, nozzle leaks, or open pouring, the entrapment of air argon bubbles and solid inclusion particles in the solidifying shell, entrainment of mould slag, surface defects and breakouts due to level fluctuations, inadequate liquid slag layer coverage, meniscus stagnation, and jet impingement. Low in the caster, fluid flow is a critical contributing factor to macrosegregation, such as centreline segregation, intergranular segregation, and other problems.

In slab casting, the mould flow pattern varies between two extremes:

— With an upward directed jet exiting the nozzle or a large amount of argon gas injection, the flow will quickly reach the top surface and travel away from the nozzle towards the narrow faces before being turned downwards. This "single roll" flow pattern is more likely with multi-port nozzles, or bifurcated nozzle with small, upward-directed ports. It is also encouraged by shallow nozzle submergence, low casting speed, or large mould widths. Surface velocities and level fluctuations are high, so mould slag entrainment and surface defects are likely.

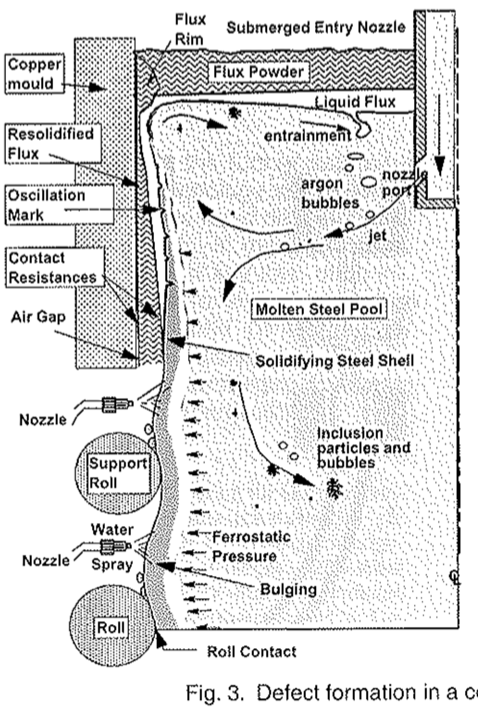
— With the other typical mould flow pattern, the steel jet enters the mould cavity from a more deeply-submerged nozzle with larger or downward-angled entry ports of a bifurcated nozzle. The submerged jet then travels across the width of the mould to impinge on the narrow faces. The jet then splits. Some of the flow travels upward towards the meniscus and back across the top surface towards the nozzle. The rest of the jet flows down the narrow faces deep into the liquid pool. Two large recirculating regions are formed in each symmetric half of the caster, so this flow pattern is termed "double roll". Often, the flow pattern alternates between the single and double roll archetypes or it may attain some intermediate condition.

The flow pattern in a given continuous casting mould can be determined in several different ways. Traditionally, understanding has been deduced from physical models constructed to scale from transparent plastic using water to simulate the molten steel. Water models have proven to be accurate for single phase flows regardless of the model scale factor, so long as the flow is fully turbulent. Obtaining accurate flow patterns is very difficult when gas injection is significant, and some phenomena, such as slag layer behaviour, cannot be modeled quantitatively, owing to the inherent differences in fluid properties, such as density and surface tension.

Mathematical models can yield added insight into flow. Computational models based on finite-difference or finite-element solution of the Navier-Stokes equations can include phenomena such as heat transfer, multiphase flow, and solidification in steel casting without the inaccuracies inherent in a water model. Accurate calculations still require significant effort because these models need accurate property data, appropriate boundary conditions, numerical validation, experimental calibration, and a lot of computer time.

Flow can also be measured directly in the actual steel caster, but due to the complicated conditions the above mentioned methods are more common.

As an example, Fig. 4 shows a typical double-roll flow pattern modeled in the mould region of a continuous slab caster[37]. The right side visualizes the flow using particle image velocimetry. In order to get good resolution in the PIV measurements, images were recorded in several different regions and combined to form a compo-



Defects in Continuous Casting

Surface defects from:
- Level fluctuations
- Meniscus freezing
- Poor flux infiltration

Internal defects from:
- Inclusions
- Flux entrainment

Cracks from:
- Thermal stress
- Bulging, etc.
- Metallurgical embrittlement

Fig. 3. Defect formation in a continuous casting machine

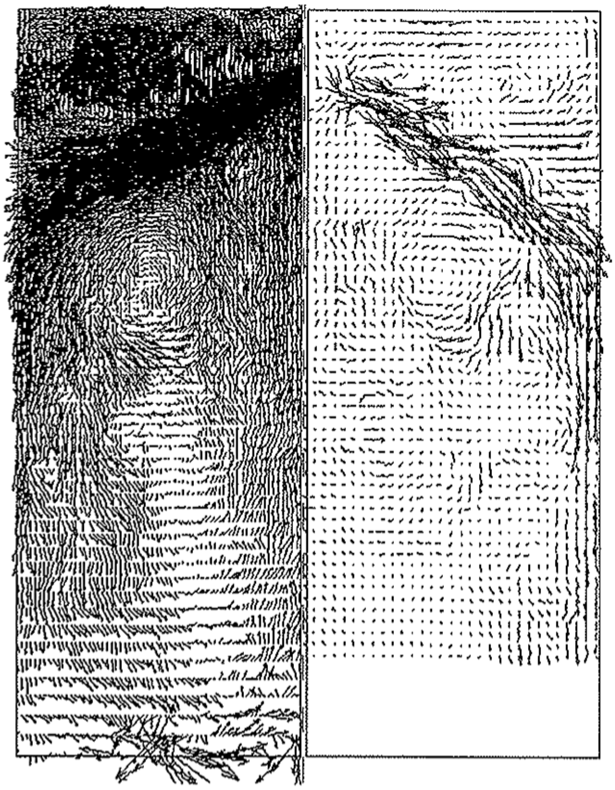


Fig. 4. 3D Large Eddy Simulation (left side); particle image velocimetry (right side)

site picture. The symmetrical left side shows velocities calculated from a transient DNS simulation of 3-D turbulent flow[38].

A typical three dimensional fluid flow model solves the continuity equation and Navier-Stokes equations for incompressible Newtonian fluids, which are based on conserving mass (one equation) and momentum (three equations) at every point in a computational domain[10, 39]. The solution of these equations, given elsewhere[38], yields the pressure and velocity components at every point in the domain. At the high flow rates involved in this process, these models must incorporate turbulent fluid flow. Many different turbulence models have been employed by different researchers for fluid flow in continuous casting, such as effective viscosity models[40, 41] (for the cylindrical mould and straight nozzle), one equation turbulence models (turbulent energy K plus a given length-scale)[42], two-equation turbulence models such as the K-ε Model[43, 44], LES (Large Eddy Simulation)[45–47], possibly with a SGS (sub-grid scale) model[48, 53], and DNS (direction numerical simulation)[38].

Among these models, direct numerical simulation is the simplest yet most computationally-demanding method. DNS uses a fine enough grid (mesh), to capture all of the turbulent eddies and their motion with time. To achieve more computationally-efficient results, turbulence is usually modeled on a courser grid using a time-averaged approximation, such as the popular K-ε model, [44], which averages out the effect of turbulence using an increased effective viscosity field, μ_{eff}. This approach requires solving two additional partial differential equations for the transport of turbulent kinetic energy and its dissipation rate[38]. The standard high-Reynolds-number K-ε model generally uses assumed "wall functions" to capture the steep gradients at wall boundaries, in order to achieve reasonable accuracy on a course grid[44, 49, 50]. Alternatively, the low-Reynolds-number turbulence model treats the boundary layer in a more general way, but requires a finer mesh at the walls. Large eddy simulation is an intermediate method between direct numerical simulation and K-ε turbulence models, which uses a turbulence model only at the sub-grid scale[45–47].

2.2 Phase Transformation and Segregation

The phase transformation from liquid to solid is one of the most comprehensive treated physical phenomena. Numerous methods and techniques are in use, which to discuss in detail would go far beyond the scope of this work. In the following, only the basic approaches for the two most important resolution methods, the finite difference method (FD) and the finite element method (FE) will be introduced.

The general differential equation for the variable Φ can be written as follows[10]:

$$\frac{\partial}{\partial t}(\varrho\Phi) + \mathrm{div}(\mathrm{pu}\Phi) = \mathrm{div}(\Gamma \mathrm{grad}\Phi) + S \qquad (1)$$

where Γ is the diffusion coefficient, and S is the source term.

Neglecting the transport term and setting the source term to

$$S = L\,\frac{\partial f_s}{\partial t} \qquad (2)$$

(with f_s the solid fraction), Eq. (1) can be written as

$$\varrho c_p \frac{\partial T}{\partial t} = \mathrm{div}(\varkappa\,\mathrm{grad}T) + L\,\frac{\partial f_s}{\partial t}, \qquad (3)$$

where ϰ is the thermal conductivity, ϱc_p is the volumetric specific heat and L the volumetric latent heat of transformation. The volumetric enthalpy H is defined as:

$$H = \int_0^T \varrho c_p(T)dT + L(1 - f_s). \qquad (4)$$

This leads to:

$$\frac{\partial H}{\partial t} = \varrho c_p \frac{\partial T}{\partial t} - L\,\frac{\partial f_s}{\partial t}. \qquad (5)$$

Combining Eq. (3) and (5) gives:

$$\mathrm{div}(\varkappa\,\mathrm{grad}T) = \frac{\partial H}{\partial t} \qquad (6)$$

The enthalpy is a continuous function of the temperature T, except at the melting point of a pure metal (or at the eutectic temperature). For numerical simulation of heat transfer phenomena it is most common to solve the heat transport equation like given in Eq. (6), typically called the enthalpy method[11].

The Finite Element formulation of Eq. (6) leads to the following set of non-linear differential equations:

$$[M]\,\frac{\partial H}{\partial t} = -[K]\,T + b \qquad (7)$$

where T and H are the vectors containing the unknown temperatures and enthalpies at the nodes, respectively, [M] is the mass matrix, [K] is the so-called stiffness matrix and b contains the contributions of the boundary conditions.

An explicit time stepping scheme would give:

$$[M]\,\frac{H^{(n+1)} - H^{(n)}}{\Delta t} = -[K]\,T^{(n)} + b. \qquad (8)$$

From temperatures and enthalpies at time t_n, the enthalpies at time t_{n+1} can be calculated by solving system (8), T_{n+1} can be computed by using the relation T(H).

The use of an implicit scheme gives:

$$[M]\,\frac{H^{(n+1)} - H^{(n)}}{\Delta t} = -[K]\,T^{(n+1)} + b. \qquad (9)$$

The success in applying implicit schemes is based on maintaining the accuracy in the results, while at the same time avoiding excessive iterations in the solution of the resulting non-linear equations. Under several implicit schemes, the general enthalpy method proposed by Swaminathan and Voller[12] has to be mentioned as efficient and accurate.

As the solidification of steel under practical conditions is far away from equilibrium, segregation in the macro- and microscopic scale plays an important role. Microsegregation develops at the scale of dendrites, macrosegregation on the scale of the casting. In recently published work, M. Flemings[30] and C. Beckermann[31] review the understanding and modelling of macrosegregation. Basically, the cause of macrosegregation is long-range advection of alloy species due to the relative movement or flow of segregated liquid and solid during solidification. In continuous casting, the feeding of solidification shrinkage, applied magnetic fields (stirring), movement of dendrite fragments, and the deformation of the solid network due to stresses (e.g. bulging) are the main reasons for macrosegregation. Macrosegregation modelling in ingot casting (e.g. [32]), single-crystal casting (formation of freckles in superalloys) (e.g. [33]), or die casting[33] reached a high level during recent years (e.g. development of coupled microstructure-macrosegregation models[31]). In continuous casting of steel, the influence of soft reduction and bulging on macrosegregation have been the most treated subjects[30].

In microsegregation modelling, many theoretical approaches and models exist, too. For several reasons, microsegregation is not that important and often investigated question in conventional continuous casting of steels. The main reason is, that for a given steel composition, the operating window of the caster is so small, that the microsegregation cannot be significantly influenced. Furthermore, the reheating and deforming of the strand leads to a partial homogenization of the final product. This reduces the influence of microsegregation on the mechanical properties of the final product. The current trend towards strip casting and thin slab casting, associated with high cooling rates and decreasing deformation degree will make the question of microsegregation much more interesting.

Segregation plays an important role in the formation of internal cracks during solidification. Microsegregation leads to an interdendritic enrichment of heavy segregating elements, and a widening of the so-called Brittle-Temperature-Range I (BTR I, the temperature range between zero-strength and zero ductility temperature). An overcritical deformation of the dendritic structure results in crack initiation at the scale of dendrites. During crack growth, macrosegregation plays an important role, too (suction of enriched melt). Figure 5 shows a concentration mapping (CM) of a segregated internal crack in a 0.089 % C steel. The length of the present crack is more than 2 mm; cracks in cast products can grow even longer. Internal cracks can become macrosegregation defects, as the alloy concentration within the crack may produce more serious problems in the final product than the crack itself. Crack initiation depends on microsegregation. Microsegregation calculations provide a suitable tool for the qualitative indication of the influence of alloying elements on internal crack susceptibility[35,36]. The enrichment of phosphorus (P), for example, depends on C-content. The lower equilibrium partition coefficient between austenite and melt compared with ferrite and melt, and the higher back diffusion in ferrite lead to higher P enrichment in the interdendritic melt with increasing C content, Fig. 6, which results in widening of BTR I. A correlation with the results of hot tensile tests shows[35], that P is much more harmful in peritectic and hyperperitectic middle and high carbon steels, than in hypoperitectic, low carbon steels.

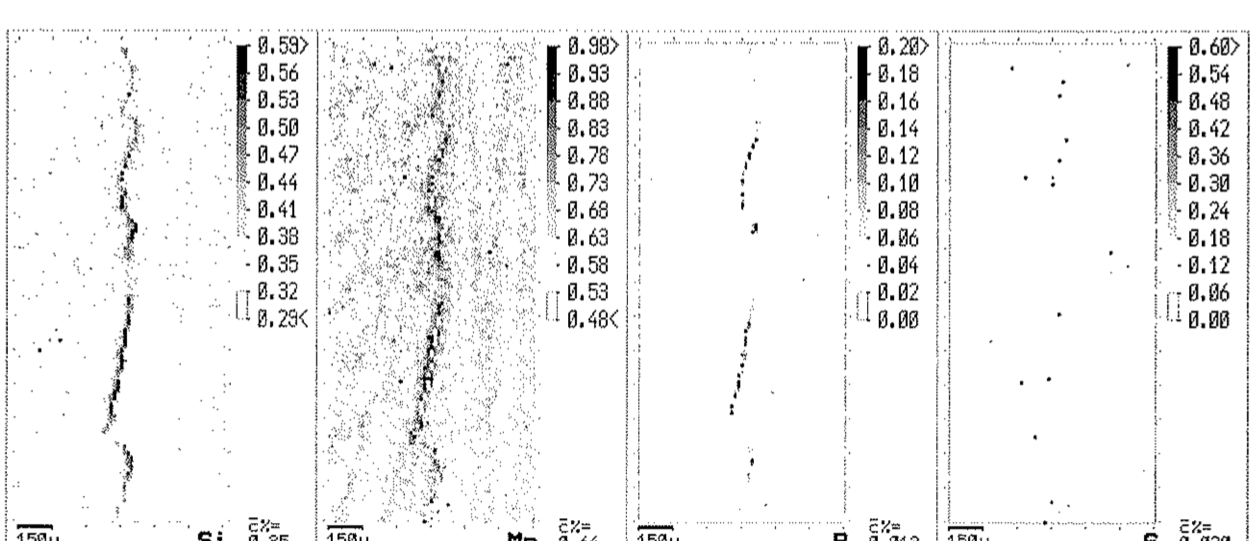


Fig. 5. Concentration mapping (CM) of segregated crack in a steel with 0.089 % C, 0.41 % Mn, 0.011 % P and 0.012 % S

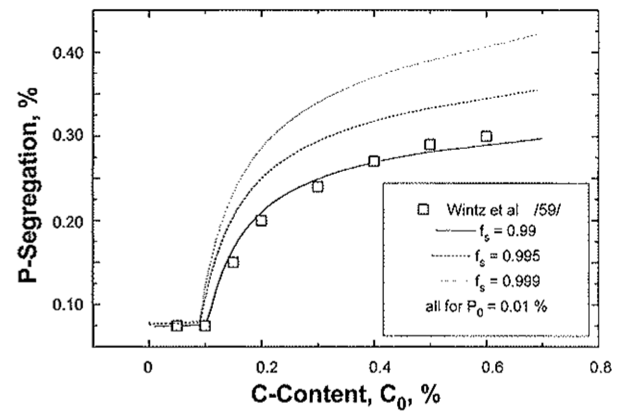


Fig. 6. P enrichment versus C content for initial P content of 0.01 %

2.3 Microstructure Simulation

The traditional method of predicting microstructure in casting is based on the measurement of structure parameters, like dendrite spacing or grain size in correlation with solidification parameters, like cooling rate (dT/dt), thermal gradient (G) or growth velocity (R). The microstructure length scale includes phase spacing as a function of cooling rate $\lambda = f(dT/dt)$, or as a function of thermal gradient and growth velocity $\lambda = f(G,R)$, and it also includes grain density as a function of nucleant efficiency (contact angle Θ) and cooling rate, $N = f(\Theta, dT/dt)$.

As discussed by D. M. Stefanescu in two review papers[3,4], the cooling rate results from the coupling of macro heat transfer from the strand to the environment with the heat evolution during solidification, which is dictated by transformation kinetics. If the transformation kinetics are independent from the macro heat transfer, the calculations can be performed uncoupled. In most classic macro-transport models, T is evaluated from macro heat transfer, and λ and N are calculated from empirical equations as a function of dT/dt.

In recent years the development of coupled macro heat transfer – transformation kinetics codes forged ahead. Both stochastic and deterministic models have been proposed. Compared with deterministic models the mathematics of stochastic models are relatively simple[3]. Deterministic models are based on the solution of the continuum equation at two different length scales, macro and micro. The transformation kinetics have to be coupled with the macro-transport. Several numerical methods have been developed to perform these calculations[3].

Whereas stochastic approaches for microstructure evolution in typical casting alloys gain more and more currency, the simulation of microstructure in the continuous casting of steel is still a new area for the following reasons:

- Steels typically undergo solid state transformations after solidification. This and the fact, that continuous cast material is further deformed makes the solidification microstructure less important for the final product properties.
- The conventional continuous casting process gives only a small operating window. Within this window and for a given steel composition, the microstructure cannot be significantly influenced.

Only now, since the development of thin slab and thin strip casting with increasing cooling rate and decreasing deformation degree the simulation of microstructure becomes more attractive for steel producers[5].

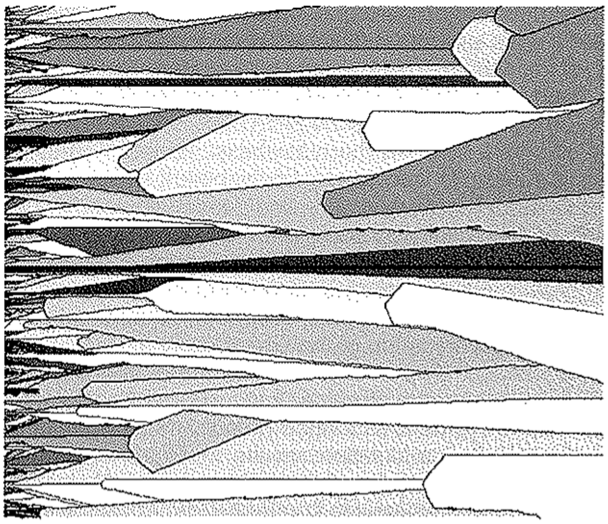


Fig. 7. Microstructure simulation for fictive alloy, different gray tones correspond with different cristallographic orientation

An important advantage of stochastic models is, that crystallographic effects on the growth and selection of dendritic grains are considered, and the grain structure becomes visible. Two techniques are presently used for stochastic modelling of solidification, the Monte Carlo (MC) technique, and the Cellular Automaton (CA) technique, the second one to be described more detailed. Rappaz and Gandin[6–8] applied the CA technique to the simulation of grain structure formation in solidification processes. The model includes the mechanisms of heterogeneous nucleation and of grain growth. Nucleation occurring at the mould wall as well as in the liquid metal are treated by using two different Gaussian distributions of nucleation sites. The characteristics of these two distributions, the mean undercooling ΔT_{max}, standard deviation ΔT_0 and total density of grains n can only be determined via experimental observations. The location and the crystallographic orientation of the grains are chosen randomly among a large number of cells and a certain number of orientation classes, respectively. The growth kinetics of both columnar and equiaxed morphologies can be calculated with the aid of the Kurz-Giovanola-Trivedi (KGT) model[9]. It is assumed, that the growth velocity R depends on the dendrite tip undercooling as follows:

$$R = a_2 \cdot \Delta T^2 + a_3 \cdot \Delta T^3.$$

The preferential growth directions of cubic metals are taken into account. The columnar-to-equiaxed transition (CET), the selection and extension of columnar grains which occur in the columnar zone and the impingement of equiaxed grains can be shown by this technique. Figure 7 gives an example of the evolution of microstructure of a fictitious alloy.

3. Examples for Modelling of Defect Formation and Material Properties in CC

3.1 Defects from Level Fluctuations

Thermal-mechanical models can be applied to understand the mechanism(s) governing the evolution of various defects in the process. As an example, such a model was used to simulate defect formation during a level fluctuation. The transient temperature histories calculated in a longitudinal section through the steel shell at the meniscus region is coupled with an elastic-visco-plastic finite-element thermal stress model to simulate the deformation and stress development of the shell[51].

A sudden severe drop in liquid level exposes the inside of the solidifying shell to the mould slag, and also leads to surface depressions. Relaxing the temperature gradient causes cooling and bending of the top of the shell toward the liquid steel. When the liquid level rises back, the solidification of new hot solid against this cool solid surface layer leads to even more bending and stresses when the surface layer reheats[51]. This sequence of events is illustrated on a 20 mm long section of shell in the calculation results in Fig. 8, for a 20–30 mm level drop lasting 0.6 s[51]. When liquid steel finally overflows the meniscus to continue with ordinary solidification, a surface depression is left behind. The event is accompanied by significant transverse tensile stress, which could lead to longitudinal cracks. Thus, the model is able to illustrate how transverse depressions and longitudinal cracks might be found together.

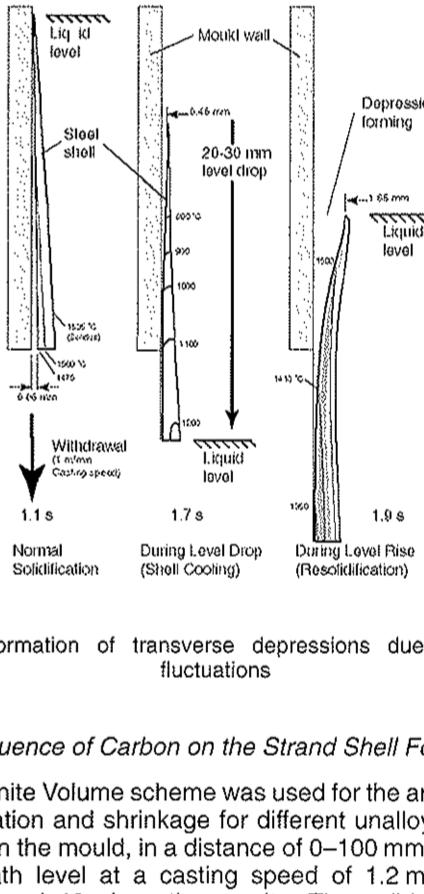


Fig. 8. Formation of transverse depressions due to level fluctuations

3.2 *Influence of Carbon on the Strand Shell Formation*

A 1D Finite Volume scheme was used for the analysis of solidification and shrinkage for different unalloyed steel grades in the mould, in a distance of 0–100 mm from the steel bath level at a casting speed of 1.2 m/min. Figures 9 and 10 show the results. The solid fractions $f_s = 0.8$ and 1 are termed here as zero strength solid fraction and zero ductility solid fraction . The δ-γ-phase transformation has a main influence on the shrinkage of steels during solidification. Depending on the carbon content of the steel, the δ-γ-phase transformation occurs during or immediately after solidification for steels with less than 0.5 mass-% C. The influence of C-content on steel solidification and shrinkage can be summarized as follows[22]:

- δ-γ-phase transformation occurs earlier with higher C-content; for C < 0.1 mass-%, it occurs in the completely solidified state ($f_s = 1$), and has its largest range at C = 0.1 mass-%. For C from 0.1 to 0.16 mass-% the δ-phase transforms in the brittleness range, and for steel grades with C = 0.16–0.50 mass-%, it transforms at temperatures which correspond to f_s of about 0.8.
- Irregular shell growth can be observed for steel grades with C = 0.042, 0.1 and 0.135 mass-%; a regular growth at C = 0.18 and 0.57 mass-%.
- The strength of steel with C-contents < 0.1 mass-% increases with higher C-content. This is due to the higher austenite fraction. The strength and stiffness of a steel shell with C-contents > 0.1 mass-% decreases with increasing C-content because the shell has a higher liquid fraction.

For steel with C-contents <0.16 mass-%, the effect of shrinkage increases with higher C-content while at the same time the effect of stiffness decreases for C-contents between 0.1–0.16 mass-%. At 0.12 mass-% this overlapping may be the cause of nonuniform shell growth.

Some of these results are well known from continuous casting practice. In order to validate the results quantitatively, an experiment method was developed, as described in detail elsewhere[35, 36]. The so-called Submerged Split-Chill Tensile test method allows the measurement of shrinkage during solidification at controlled cooling conditions. Figure 11 shows the shrinkage force for a

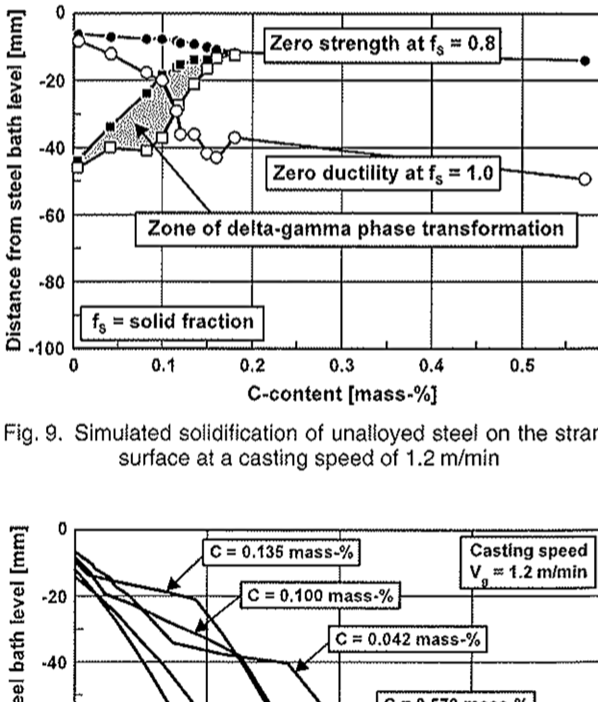


Fig. 9. Simulated solidification of unalloyed steel on the strand surface at a casting speed of 1.2 m/min

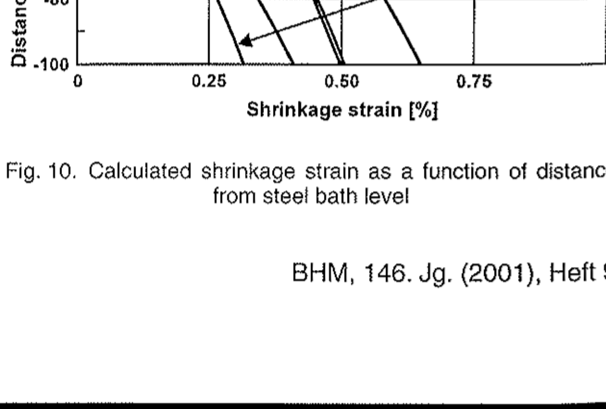


Fig. 10. Calculated shrinkage strain as a function of distance from steel bath level

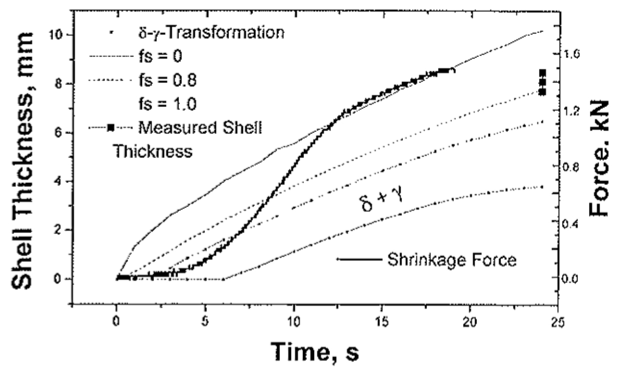


Fig. 11. Measured shrinkage force versus time with shell growth and δ/γ-transformation range

0.081 % C, 0.27 % Si and 1.53 % Mn steel grade, together with the calculated shell growth, and the δ-γ-phase transformation range during the first 20 s of solidification. The measurements yield some new perspectives: the shrinkage curves for every steel grade have reproducibly a typical shape. For low carbon steels for example, the force decreases after reaching a maximum, although, only a few cracks have been found in the metallographic examination. This behaviour is difficult to explain. The same behaviour can be obtained for steels with 0.2 % C, which appear very crack sensitive. For steel grades with less than 0.1 % C, but near the onset of peritectic reaction a steadily increasing shrinkage force can be obtained. With exceeding 0.1 % C, the shrinkage force reaches a maximum value, and remains constant until the end of the test. This points at an influence of primary creep and dynamic recovery (even if this should not be expected after such a short time). The results will be the basis for a further analysis, under consideration of creep laws in thermo-mechanical models. Mould taper optimization seems an applicability for the future.

3.3 Micromechanical Modelling of the Hot Ductility of Steel

For more than a decade research and engineering interests have been evident in advanced materials such as metal matrix composites, functionally graduate materials or laminates, which are highly inhomogeneous at some microscale and consist of at least two constituents (or "phases") different in the individual material properties. Micromechanical modelling aims to describe the thermomechanical behaviour of inhomogeneous materials by using continuum mechanical methods and by explicitly accounting for the material properties and geometrical arrangements of the constituents. Because spatial variations of the mechanical behaviour of realistic microscale structures can hardly be captured computationally, many descriptions of multi-phase materials are based on Mean Field Approaches (MFA), Periodic Microfield Approaches (PMA) or Embedding Methods, which are generally integrated in Finite Element codes.

In more recent time the iron and steel research society is also considering these micromechanical tools for detailed analysis with respect to material design, study of the overall mechanical properties and damage analysis. Related publications can be found for e.g. HSS-grades, dual phase steel, IF-grades and steel at phase transformation temperatures, compare[52–54], the utilization PMA is demonstrated to study the basic damage reasons at phase transformation temperatures typically occurring during continuous casting of steel. The PMA are most suitable for material characterization and for predicting phase arrangement effects in the initiation of local damage of real multi-phase materials obtained by computing the displacements, strains and stress distribution considering suitable periodic microstructures within these materials. For a comprehensive description on micromechanical methods see, e.g.[55,56].

At temperatures close to the austenite – ferrite phase transformation, carbon steel typically exhibits a loss of ductility and a tendency to intercrystalline cracking. One of the major causes for this behaviour is the precipitation of ferrite, which is much softer at these temperatures in comparison to austenite. This ferrite starts to precipitate along the primary austenite grain. To study the mechanical response of such a microstructure to external loading conditions, a regular arrangement of columnar austenite grains is modelled by 2-dimensional unit cells as presented in Fig. 12. The grey regions represent two quarter pieces of hexagonal austenite grains while the white regions represent the growing ferrite, respectively. In accordance with experimental observations the model simulates a statistically higher ferrite volume fraction at the austenite grain boundaries. Employing symmetry conditions at the boundary of the unit cell (e.g. this pattern is periodically repeated in all directions) and introducing a generalized plain strain condition provides a reasonable model for the columnar microstructure (i.e. the length of the grains exceeds several times the diameter) of primary austenite found close to the surface of a cast steel.

With these kinds of models it is feasible to give quantitative answers to questions on the strain concentration at the grain boundaries due to global mechanical deformations, on strain rate dependencies of the stress and strain fields and consequently on the ductility and damage behaviour of steel at high temperatures.

In[28,57] it is demonstrated that depending on the amount of transformed ferrite, local strains close to the austenite grain boundaries can exceed the global (macroscopic) strains several times as indicated in Fig. 13, which exhibits the strain concentration at the former austenite grain boundaries applying a global uniaxial strain ε_{11} of 1 %.

Coupling such thermo-mechanical models with numerical thermodynamic models, which are able to describe the thermodynamic stabilities of the individual constituents, allows to study the impact of global mechanical loading conditions on the phase transformations and

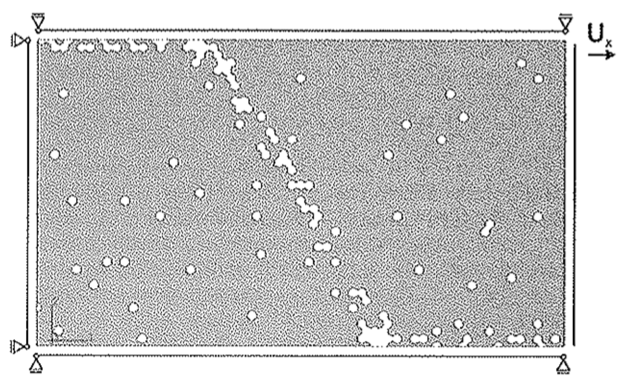


Fig. 12. FE-Model: austenite-ferrite phase arrangement with a volume fraction of 5 % ferrite

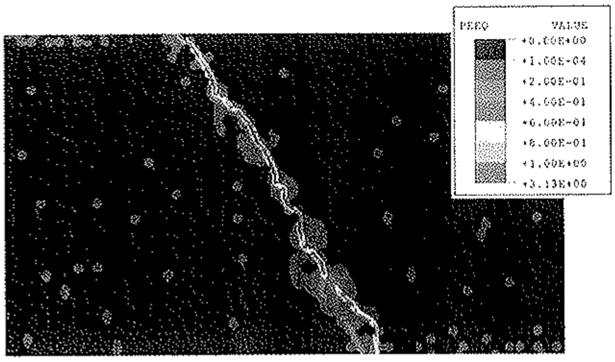


Fig. 13. Equivalent plastic strain at the micro scale due to a global strain of $\varepsilon_{11} = 0.01$. The global strain is compensated by large local strains in the softer ferrite films

vice versa the influence of phase transformations on the local stress and strain fields. This is the topic of ongoing research, compare e.g.[57,58]

4. Summary

The present paper provides an overview of the application of numerical modelling to the optimization and further development of continuous casting. The basic physical principles and some of the issues in the coupling of models in different length scales are described. A multi-physical approach will be the challenge for the future. Some selected examples demonstrate the power of the new technique, and the potential for the future.

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Mikrostrukturelle Modellierung der Warmumformung

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Zielsetzungen der mikrostrukturellen Warmumformsimulation – Mikrostrukturelle Vorgänge im Zuge der Warmumformung – Semi-empirische und physikalische Gefügemodelle – Wechselwirkungen zwischen Ausscheidungs- und Rekristallisationskinetik – Prozessmodelle für das Walzen von Flach- und Langprodukten – Schmiedesimulation und Kopplung der Gefügemodelle mit Finite-Elemente-Programmen – Entwicklungsbedarf bezüglich Vorhersagegenauigkeit und Anwendungsbreite

Microstructural Modelling of Hot Forming. Objectives of microstructural modelling of hot forming processes – Microstructural phenomena during hot forming – Semi-empirical and physical description of microstructural development – Interactions between precipitation and recrystallization kinetics – Process models for hot rolling of flat and long products – Forging simulation and coupling of microstructural models with finite element programs – Need for further developments regarding accuracy of prediction and broader applicability

1. Einleitung

Mit der zunehmenden Leistungsfähigkeit moderner Computer ist es seit einigen Jahren möglich, die eigenschaftsbestimmenden mikrostrukturellen Vorgänge im Zuge der Warmformgebung in Prozessmodelle, wie beispielsweise für das Walzen, Freiformschmieden, Gesenkschmieden oder Strangpressen, zu integrieren[1-3]. Dadurch kann die Wirkung der Prozessparameter auf die Gefüge- und Eigenschaftsentwicklung ursachengerecht und mit Einbeziehung der Wechselwirkungen sehr genau ermittelt werden. Daraus resultieren einerseits bessere Werkstoffe und andererseits kann der Umformprozess offline optimiert oder über die Kopplung mit der Anlagentechnik direkt gesteuert werden. Durch dieses Konzept ist es möglich, neben der gezielten Änderung der Form auch eine gewünschte Beeinflussung der Gefügeausbildung und damit verbunden der Bauteileigenschaften zu erreichen. Durch die modellbasierte Kontrolle thermo-mechanischer Umformvorgänge können

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