Modelling Solidification in Continuous Casting: Algorithms and Boundary Conditions

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ABSTRACT: The application of numerical methods for an increased understanding and optimisation of the continuous casting process has substantially gained in importance during the past decades. One of the key issues is the coverage of the solidification conditions by numerical models, which is the basis for all subsequent metallurgical analyses of e.g. micro-structure or segregation phenomena. In the following paper some the essential aspects for the compilation of such process-related solidification models will be highlighted: On the one hand, efficient multi-dimensional process modelling requires the use of special algorithms in order to minimize computing time – a possible algorithm, which is not covered by the classic finite difference/element methods, will be described. On the other hand, realistic solidification models which accurately reproduce the thermal conditions during the casting process necessitate a broad acquisition of boundary conditions, which are usually unique for each caster. Therefore, some well suited methods for obtaining reliable boundary conditions for all zones of the caster will be presented. Lastly, an overview on proven techniques for validating the modelling results will conclude the paper.

1. INTRODUCTION

Research development as well as industrial process optimisation of the continuous casting processes – being the key solidification process in steelmaking – nowadays often requires numerical descriptions of the different metallurgical phenomena in the process. These occurrences, which can for example include hot tearing, surface cracking, inclusion entrapment, oscillation mark formation, micro- and macrosegregation or phase transfor-mations, have been subject of an uncountable number of research studies. The individual treatment of these aspects by physical as well as numerical models has been published, however a comprehensive combination of the singular models together with the actual solidification conditions in a caster has still not been fully addressed.

Since nearly all of these models need input parameters resulting from macroscopic solidification models (e.g. temperature, temperature gradient, shell thickness, growth velocity, …) correct and validated as well as comprehensive numerical descriptions of casting machines are the essential basis for the previously mentioned goal. In the past, several groups have taken up the objective of creating (transient) numerical solidification models – sometimes with the purpose of real-time control of the caster, thus necessitating simplifications: Louhenkilpi, Miettinen and co-workers[e.g. 1,2] published a multi-dimensional transient heat transfer model called TEMPSIMU3D with the special feature of applying a non-linear solid fraction vs. temperature relationship computed by the IDS model[3,4]. Spitzer et al.[e.g. 5] present a model aimed at controlling dynamic spray cooling by tracking slab slices. A similar aim was pursued by Hardin, Beckermann et al.[e.g. 6] in their DYSCOS model. Finally, Thomas and co-workers[e.g. 7] have developed the CON1D and CON2D models for different continuous casting simulations, partially coupling the thermal simulations with stress models. However, most of the mentioned publications only give rare information on the determination of the thermal boundary conditions, which can be regarded as equally important as the algorithm methodology.

Thus, the aims of the present paper are twofold: Firstly, a transient two-dimensional approach for the computation of the temperature distribution in the strand is shown, which has been developed under the viewpoint of minimised computation time and sufficient accuracy. Secondly, some possibilities of determining thermal boundary conditions in different sections of the caster (mould area, secondary cooling zone) together with methods for validating the results directly at the caster will be contrasted.

2. ALGORITHM DESCRIPTION, FORMULATION AND EVALUATION

Generally, the solution of every problem of heat conservation is based on the conservation of energy in a selected volume. Inserting FOURIER's law as a constitutive equation for energy yields the following parabolic differential equation,

$$\frac{\partial}{\partial t}\left(\rho H(\vartheta)\right) = \nabla \cdot \left(\kappa(\vartheta)\mathbf{grad}\,\vartheta\right) \tag{1}$$

where $t, \rho, H, \vartheta, \kappa$ are time, density, enthalpy, temperature and thermal conductivity, respectively. The LHS accounts for transient effects while the RHS accounts for heat conduction in n directions; convection effects are neglected. The treatment of the transient term, which requires a relationship between enthalpy and temperature and possibly a consideration of latent heat of fusion will be treated later on in the paper.

Since an analytical treatment of Eq. (1) would require several simplifications, the solution to Eq. (1) can only be obtained numerically by discretising the numerical quantities over a defined number of points. With the exception of beam blank casting, simulations of continuously cast products are relatively simple regarding their computational domain, meaning that no complex geometrical conditions need to be considered. Thus, the scope of possible numerical methods is not only limited to those of the finite element methods – the use of finite differences/volumes methods is likewise also a possible choice. A comprehensive description of the basics of these numeric methods can be found in the literature[8].

Seeing that computational effort is a substantial criterion in the present study, a careful choice of the numerical methods has to be done. As differences in runtime will be unobservable for the 1-dimensional case, only multidimensional problems should be discussed: Here the selection of discretisation method (finite element vs. finite difference/volume) linked with the appropriate subsequent solver can actually influence the result significantly. In the present 2-dimensional study, the alternating-direction implicit method has been chosen as an effective finite difference/volume method.

2.1 The Alternating-Direction Implicit (ADI) Method

In the late 1950s, Douglas, Peaceman and Rachford published a novel idea of treating multidimensional, elliptic or parabolic differential equations by numeric means in a finite difference model[9,10]. Their idea was to combine the advantages of an explicit handling (no system of linearly dependent equations) with those of an implicit method (unconditional stability). While a fully explicit treatment of a such natured problem would be strongly impaired by the conditional stability due to limited time and mesh spacing, the fully implicit method of a domain with $I \times J$ nodes would yield a system of $I * J$ equations with 5 non-zero diagonals in matrix formulation, requiring considerable computational effort for its solution.

The authors of the ADI method propose to split one computational step into two »semi-implicit« half steps. As shown in Fig. 1, where the superscript n denotes the time-step indexing, at first one calculation direction is treated implicitly and the other explicitly (step $n+1/2$). In the second half step (step $n+1$), the explicit/implicit assignment is switched between the two calculations. In short, the following benefits of such handling can be summarized:

- Due to the semi-implicit treatment, unconditional stability is retained.
- In the ADI approach $2(I * J)$ equations, however only with 3 non-zero diagonals, need to be solved. The necessary computational effort is substantially lower than that of the fully implicit formulation.

2.2 Treatment of Solidification-Related Aspects

Regarding the applicability of the ADI method to solidification problems, two key issues can be defined: Firstly, the treatment of temperature dependent material properties and secondly the consideration of latent heat of fusion. In the present study, the first question was solved by introducing an overrelaxation technique[11].

In order to accurately account for the latent heat of fusion, it is suggested to use the *effective specific heat method* by reformulating the LHS of Eq. (1) to

$$\frac{\partial}{\partial t}\left(\rho H(\vartheta)\right) = \rho c_p^{eff}(\vartheta)\frac{\partial \vartheta}{\partial t} \qquad (2)$$

where c_p^{eff} is the effective specific heat defined as:

$$c_p^{eff} = c_p + L_H \frac{\partial f_L}{\partial \vartheta} \qquad (3)$$

In Eq. (3) c_p, L_H, f_L stand for the specific heat, the latent heat of fusion and the fraction of liquid, respectively. It has to be mentioned that the term $\partial f_L / \partial \vartheta$ creates a very sharp peek in the c_p^{eff} function. Thus, unless treated with a special formulation and a wise choice of grid and time steps, large numerical errors can occur.

In order to distinguish this adapted version of the ADI method from the originally proposed one, it is proposed to call this approach the *modified alternating direction implicit (MADI)* method. A comparison of this method with analytical and other finite difference solution algorithms has already been published[12].
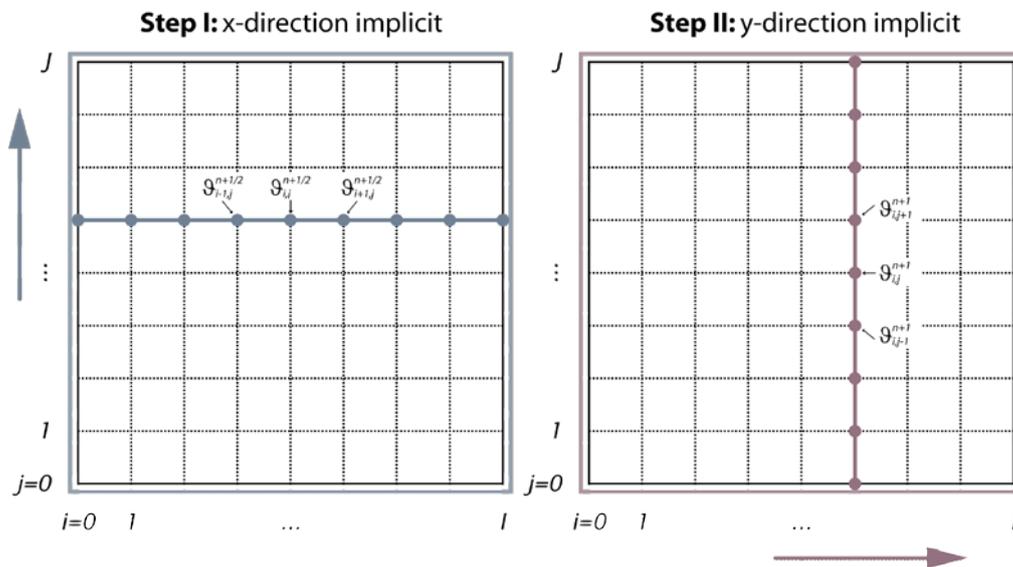
Fig. 1: General idea behind the ADI method.

2.3 Applicability Evaluation

In order to assess the applicability of the MADI method for solidification problems, a comparison with the widely accepted commercial solidification software calcosoft-2D was carried out. This software is based on the finite element method and easily allows for an implementation of temperature dependent material properties as well as the latent heat of fusion. The illustrative example which was chosen to compare the methods was the cooling of a horizontal slice of a billet caster with 100x100 mm² size. Further details on boundary conditions and material properties can be seen in Tab. 1.

Time and mesh spacing	variable
Simulation time	100 s
Material	Fe-0.6%C[1]
Starting temperature	1520 °C
Cooling	$5 \cdot 10^5$ Wm^{-2} constant on all sides

Tab. 1: Simulation Properties for Method Comparison.

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[1] The temperature dependent material properties were calculated with the software IDS16[4].

In 1984, Thomas et al.[13] published a comprehensive comparison of different modelling techniques for the special case of heat transfer problems with solidification. Among the contrasted methods are the standard finite element and the (finite difference) alternating-direction implicit (ADI) method. The authors show that the accuracy of the results in the geometrically simple case is comparable for both methods, while the computational efficiency of the ADI method is significantly better.

A similar conclusion can also be drawn from the observances of the present study which are shown in Figs. 2 and 3: Fig. 2 shows the Maximum Relative Temperature Deviation (MRTD) between the two models for all calculation steps, which is determined by the following relationship:

$$MRTD = \max\left\{ \left\| \vartheta_{i,j}^{MADI} - \vartheta_{i,j}^{calcosoft} \right\| / \vartheta^0 , \forall i,j : 1 \le i \le I, 1 \le j \le J \right\} \qquad (4)$$

It can be seen from the figure that the differences between the two methods remain negligibly small (below 0.2 %) even for medium Fourier numbers. However, it can also be seen that the results tend to differ more for increasing Fourier numbers. Since a »true« temperature can hardly be obtained for complex solidification simulations with changing material properties, no clear statement on the origin of this deviation can be made.

Regarding the runtime of the two methods, which is compared in Fig. 3, it can be concluded that the MADI method has app. $\log(N)$ runtime (N being the number of nodes) while calcosoft-2D shows app. $N \cdot \log(N)$ runtime. This fact not only becomes increasingly important for higher node numbers but also when using such a solidification model for special microstructure simulations where fine mesh spacing is required.
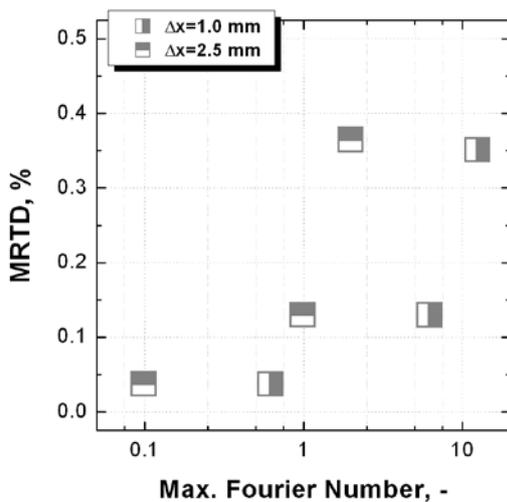
Fig. 2: Maximum Relative Temperature Deviation (MRTD) between calcosoft-2D and MADI method vs. Fourier number.
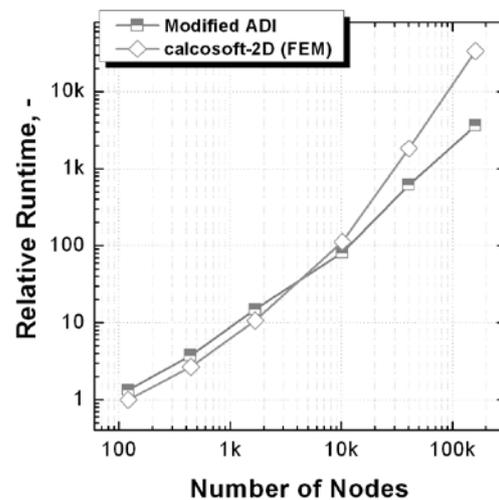
Fig. 3: Relative Runtime for calcosoft-2D and MADI for different numbers of nodes.

3. DETERMINATION OF BOUNDARY CONDITIONS

Since the results of any numerical model are just as good as the boundary conditions (BC) used, a reliable solidification model will involve obtaining ascertained and verified thermal BC for the casting machine. Moreover, the actual thermal conditions in the caster can seldom be transferred from one caster to another due to the multiple specifics of each casting machine. Furthermore, from a metallurgical viewpoint, the thermal BC will often differ depending on the cast steel grade – due to the changing behaviour of different steels, casting and cooling conditions are often changed.

3.1 Mould Heat Transfer

The heat removal in the continuous casting mould is a decisive factor for product quality and process safety. This quantity is affected by different process parameters, most

noticeably by the steel composition, the casting velocity, the mould powder and the mould taper. Although the total heat transfer between strand and mould is easily calculated from the temperature increase between primary water inlet and outlet, it only allows general conclusions on the conditions inside the mould. However, local changes in the heat transfer affect the uniformity of shell growth and in consequence the probability of surface and subsurface defect formation. The determination of the local heat transfer is rather complex, demanding the instrumentation of a mould with numerous thermocouples and subsequent inverse modelling.

In order to determine this heat transfer for a solidification model, a round bloom caster mould was instrumented with 26 thermocouples in different positions over the whole mould. By recording the temperature in the mould and subsequent elaborate inverse modelling, the differences in heat withdrawal were studied for a wide range of steel grades and casting parameters. Details on this study have already been published[14,15].

The results in Figs. 4 and 5 underline the importance of a careful and detailed consideration of the heat flux in the mould as a thermal boundary condition for solidification models. The heat withdrawal for steels – even though cast at the same casting velocity – can significantly differ depending on the steel composition. As shown in Fig. 4, a medium-carbon steel shows a very smooth decline in heat flux over the mould length while casting a high-carbon steel will lead to a remarkable increase in heat withdrawal at about 75 % of the mould length. This is attributed to the fact the strand is pressed against the mould wall in this region due to a completely different contraction behaviour of the steel. Moreover, changes in casting velocity lead to visible changes in the heat flux. Fig. 5 illustrates an increase in overall heat flux for small changes in the casting speed of app. 0.1 MWm^{-2}.
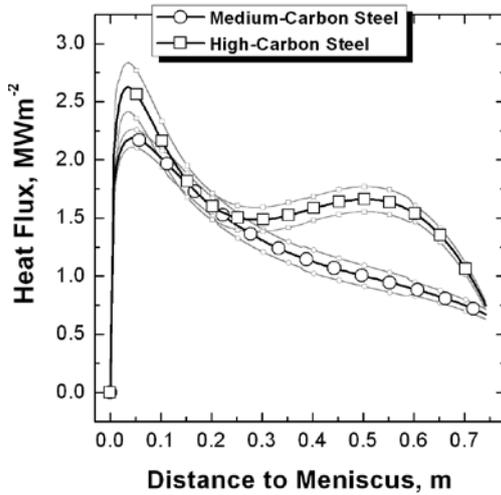
Fig. 4: Heat flux over mould length for a medium and a high-carbon steel.
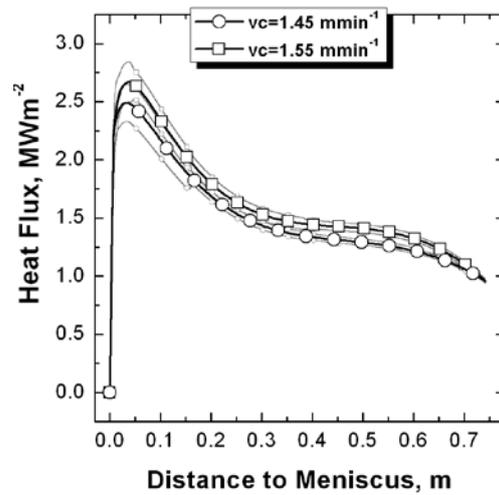
Fig. 5: Differences in heat flux for the same steel grade cast at different casting velocities.

3.2 Secondary Cooling Zone

The determination of boundary conditions for the secondary cooling zone has been subject of several studies[16–18]. Most approaches differ between a convective heat transfer by water cooling and an additional radiative term. The physics behind the radiative term is quite straightforward,

$$h_{rad} = \sigma\varepsilon\left(T_s^2 + T_{ext}^2\right)\left(T_s + T_{ext}\right)$$

(4)

where h_{rad}, T_s, T_{ext} are the radiative heat transfer coefficient, the surface temperature and the external temperature, respectively. The emissivity ε is usually a function of the amount of strand scale formation, which strongly depends on the carbon content.

Regarding the convective term several ideas have been published. Firstly, the heat withdrawal can be correlated with the water impact or the impulse of the water jet at the strand surface[e.g. 16]. A summary on this approach can be found in the literature[14]. Secondly, Wendelstorf et al.[17] and Horsky et al.[e.g. 19] have built experimental setups to determine the heat transfer coefficient of spray nozzles directly as a function of nozzle geometry, water flow rate and surface temperature. Despite the extensive measuring work, it is believed that a

nozzle specific determination of heat transfer coefficients is a promising way for obtaining reliable boundary conditions. For this reason, a measuring stand with similar aims is currently in the conception stage at the Chair of Metallurgy[20].

3.3 Possible Validation Methods

The validation of a numerical solidification model usually consists of a piecewise affirmation of results in several positions in the strand:

- Regarding the mould heat withdrawal, results from inverse modelling and temperature measurements can be compared by integral heat flux plant data (temperature record in the cooling water during the casting process). This validation step is the fundamental basis for affirming the validity of the primary part of the solidification model[13].

- Depending on their availability, breakout shells can sometimes be used to determine the shell thickness at different positions in the caster. However, as breakouts are often preceded by unsteady casting states, the application to solidification models is only limited and has to be carried out with great caution.

- In order to confirm the results of the secondary cooling zone, possibilities are twofold: Firstly, targeted defect formation (e.g. creation of white band by electromagnetic stirring or the purposeful generation of hot tears) and subsequent metallographic examination of parts of the strand is well suitable for confirming the shell thickness of the strand at certain positions. Fig. 6 shows the results of such an evaluation for the compilation of a comprehensive solidification model. In this model[14,21], the developed numerical basics were coupled with a wide choice of experiments and measurements directly at the caster. As a validation step, the strand shell thickness was determined at two different positions by artificially generating white bands (i.e. macro-segregations) in round blooms. Seeing that the values were obtained for seven different steel grades (carbon contents 0.08 to 0.8 %C) the great consistency of the model in a wide metallurgical range can be confirmed.
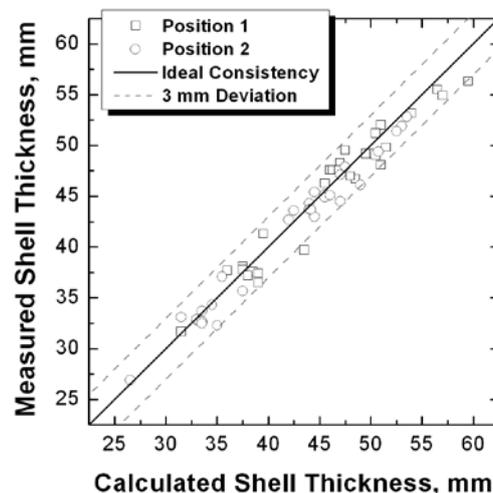
Fig. 6: Calculated vs. measured shell thickness for different steel grades at different positions for a round bloom caster[14].

- Additionally, temperature measurements by pyrometers or by dragged thermocouples can help to evaluate the surface temperature at defined points or over defined lengths of the strand. However, it has to be noted that a careful installation of the pyrometer is necessary in order to discard possible measurement perturbations by steam, next to the problems of scale formation at the surface. Regarding the use of dragged thermocouples, a careful experimental setup is necessary in order to ensure that the contact between thermocouple and strand is sufficient and well defined.

4. CONCLUSIONS

It has been outlined that the development of a numerical solidification model of a continuous caster is composed of several modules: On the one hand, algorithms for solving the energy conservation equation in the desired number of dimensions are needed. In the present paper the Modified Alternating Direction Implicit (MADI) has been introduced which is especially fit for solving multidimensional solidification problems. The comparison with a commercially available software showed that reduced computer runtime could be achieved. The second important aspect for a well-defined solidification model is the use of verified, customised thermal boundary conditions. The development of the same requires careful consideration of plant specific details, steel grade and casting parameters. In a solidification model for a round bloom caster, the precise combination of the mentioned aspects – numerics on the hand and extensive experimental boundary conditions determination on the other – has resulted in a comprehensive model which shows excellent correlation with additional validation measurements.

5. ACKNOWLEDGEMENTS

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