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EVALUATION OF APPROACHES OF NUMERICAL MODELLING OF SOLIDIFICATION OF CONTINUOUSLY CAST STEEL BILLETS

The paper evaluates two approaches of numerical modelling of solidification of continuously cast steel billets by finite element method, namely by the numerical modelling under the Steady-State Thermal Conditions, and by the numerical modelling with the Traveling Boundary Conditions. In the paper, the 3D drawing of the geometry, the preparation of computational mesh, the definition of boundary conditions and also the definition of thermo-physical properties of materials in relation to the expected results are discussed. The effect of thermo-physical properties on the computation of central porosity in billet is also mentioned. In conclusion, the advantages and disadvantages of two described approaches are listed and the direction of the next research in the prediction of temperature field in continuously cast billets is also outlined.

Keywords: steel, steelmaking, continuous casting, numerical modelling, temperature field, porosity.

1. Introduction

Continuous casting of steel is currently the main method for the manufacture of billets, slabs and blocks. During continuous casting, the steel melt is transformed in a controlled manner to the solid state of the required dimensions and shape of the cast blank designated for subsequent forming. The ladle in a continuous casting process is located on the turning stand of the casting machine. The steel is from there cast into the tundish via the ladle shroud. From the tundish, the steel is guided by submerged entry nozzles into oscillating moulds (primary cooling zone) where the "controlled" solidification of the steel is ensured. A system of the guide and support rollers is situated under the mould (secondary cooling zone) including cooling nozzles, which provide drawing, shaping and cooling of a strand of the cast steel [1,2].

It is evident that continuous casting of steel is a complex technological process, which is accompanied by a number of physicochemical processes including, for example, a multiphase flow of steel in the mould, chemical reactions (processes running between the casting powder and the melt in the mould) or the solidification (phase transition accompanied also by a change of volume with simultaneous release of the latent heat) [3,4].

In the field of production of continuously cast steel, the priority of every manufacturing company is to increase the production safety, productivity and quality of the produced steel with simultaneous minimisation of the environmental burden. Increase in productivity means an increase in the number of castings cast in one sequence without interruption of casting and subsequent restarts. On the other hand, the consecutive casting of different grades of steel requires individual adjustment of the casting parameters, in particular the casting temperature and speed in relation to the cast steel grade, and hence the cooling intensity both in the primary and the secondary zones of the continuous casting machine. The variety of process settings in relation to the cast steel grade can ultimately lead to a fluctuation and an instability of the whole system and cause thus undesirable forming of defects.

Defects of continuously cast blanks are divided into surface defects and volumetric defects [5,6]. Internal defects do not penetrate to the surface of the blank and it is therefore very difficult to detect them. The most important internal defects are:

- inclusions
- macro-segregations
- porosities
- cracks

The most important influential parameters contributing to the final quality of the blanks are the following [7,8]:

- casting speed
- casting temperature
- cooling intensity
- chemical composition of the steel

It is possible to monitor and optimize the processing parameters of the continuous casting technology and the quality of the semi-finished products by the application of physical [9]

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and mainly numerical modelling [10,11], in which numerical methods are used for solving mathematical equations of the mass transfer, movement and energy.

2. Numerical methods and computational meshes

Certain development exists in the numerical solution of equations defining flow and solidification of fluids. The oldest classical method is the finite difference method, while the finite volume method or the finite element method can be used for the solution of partial differential equations.

The principle of solution of differential equations of flow consists in covering the geometry of the solved area by a mesh and in finding a discrete solution in these sufficiently small sub-areas of basic geometry by means of the system of the so-called differential (algebraic) equations. The difference between solutions of differential and difference equations is defined as a discretization error [12].

The mesh applied to the geometry of the investigated area may be either structured or unstructured. In the first case, it is a creation of discrete non-overlapping elements where the boundary of the elements adjoins a single boundary of the adjacent element and the mesh, therefore, cannot be arbitrarily densified. At present, an unstructured mesh is being promoted, which is mainly used by the numerical finite elements method.

Both types of meshes can be constructed both in the Cartesian rectangular system (the resulting area has a shape of a rectangle or a block) and in the curvilinear system (suitable for the areas delimited by curves, circles, etc.). Examples of surface mesh elements and their own surface meshes are shown in Fig. 1a. Examples of volumetric elements of computational meshes are presented in Fig. 1b. The volumetric elements of the computational mesh are represented by the so-called hexahedrons (hexa elements), tetrahedrons (tetra elements), pentahedrons (penta elements) or wedge cells (wedge elements = triangle drawn into space) [13].

Currently, many types of simulation software exist [14] and for users it is very complicated to choose the best one for optimization of the specific process. Therefore, the paper presents the actual computational possibilities and experiences of the modelling of the qualitative parameters of the continuously cast steel billets in ProCAST simulation software based on the finite element method achieved during the solving of research projects.

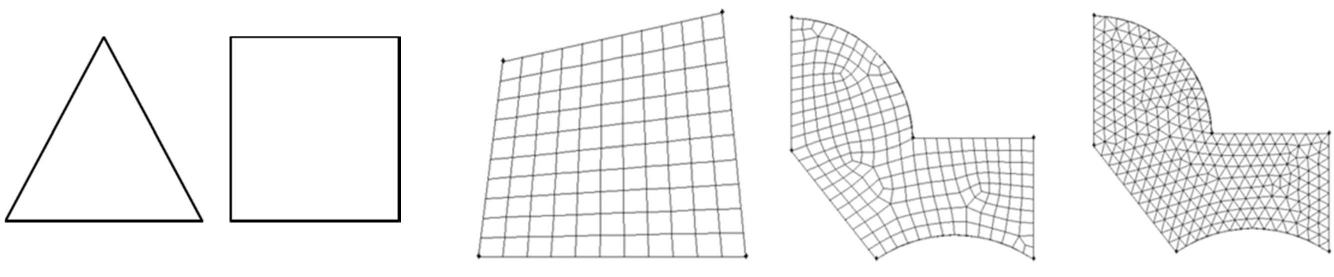
3. Approaches of numerical modelling

Generally, the algorithm of the numerical solution of each task is divided into three stages: 1) Pre-processing – it includes the geometry modelling and process of generation of the computational mesh, and definition of calculation, 2) Processing – it involves the computation in the solver, 3) Post-processing – it focuses on the evaluation of the results.

During the solving of the research projects, two approaches of numerical modelling considering the finite element method were applied using the ProCAST simulation program: the numerical modelling under the Steady State Thermal Conditions and the numerical modelling with the Traveling Boundary Conditions, which represents the non-steady state of continuous casting.

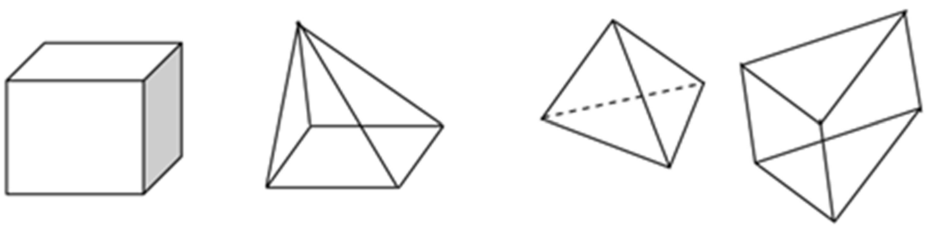
The results of both approaches must be the same although they differ in the pre-processing and processing phase, especially in the preparation of geometry, in the definition of heat transfer during the billet casting, or in the computation of the heat transfer with respect to the billet movement through the individual cooling zones. The thermo-physical properties of steel, as well as the boundary and the operational conditions, could be the same for both types of algorithms [15].

The modelling under the Steady-State Thermal Conditions is possible with the "Solid Transport" method. For the Steady-State



a) 2D surface elements

From the left: quadrangular structured mesh, quadrangular unstructured mesh and triangular unstructured surface mesh



b) 3D volumetric elements of computational mesh

Fig. 1. The examples of element shapes of: a) surface computational mesh and b) volumetric computational mesh [13]

computations, a fixed domain with mould is modelled and the solid mass is transported at the casting speed through this domain. The transport velocity of the solid mass should be tangential to the billet at each point. Knowing the casting speed and the main radius of the machine, the angular velocity is derived, as well as the angle, and finally the two components of the velocity. Both components of velocity are defined by the function vxsolidtransport.c and vysolidtransport.c using programming language C++.

Under the Traveling Boundary Conditions, a fixed domain can be also modelled, but without geometry of the mould, and the process of continuous casting is described with the use of the User Functions of Heat Flux (HF) and of Heat Transfer Coefficients (HTC). These functions define the changes of HF and HTC along the casting strand depending on casting speed for the specified section of the billet (HF for mould section, HTC for the secondary cooling zone). These functions are designated as heatflux.c and convehtransfer.c, and they are again defined in programming language C++.

A third possibility of computation under non-steady state conditions also exists. It is an approach the so-called MiLE algorithm (Mixed Lagrangian-Eulerian), which allows the possibility of having a domain, which is expanding with time, as the continuous casting process goes on. This approach, however, was not used for common numerical analysis of the process [16].

4. The Differences in Model Setup

To distinguish the differences between approaches, the 3D drawing of the geometry, the preparation of the computational mesh and the definition of the boundary conditions are outlined. Also, it is discussed the definition of thermo-physical properties of materials in relation to the expected results.

4.1. Geometry

Steady-State calculations enable to model both straight and curved continuous casting processes (including strip casting). To be close to the real process, the 3D radial shape of the strand geometry was preferred, but in the case of stress calculation, the straight geometry must be applied. The radial geometry of the modelled area of the continuous casting strand consists of the simplified mould and of the billet, which usually represents the entire curved section and also the straight section of the cast strand (see Fig. 2a). In the case of the Traveling Boundary Condition, the simplification of the geometry, which introduces only the billet as such, can be used (see Fig. 2b).

4.2. Computational Mesh

The type of the computational mesh should be prepared depending on the expected results. The hexa elements are preferred in the case of temperature field and porosity calculation (see Fig. 3a). The tetra elements must be used in the case of stress calculation (see Fig. 3b). In the case of prediction of the shell thickness at the end of the mould and the porosity, the refinement of the mesh near the surface and in the centre of the billet geometry should be considered.

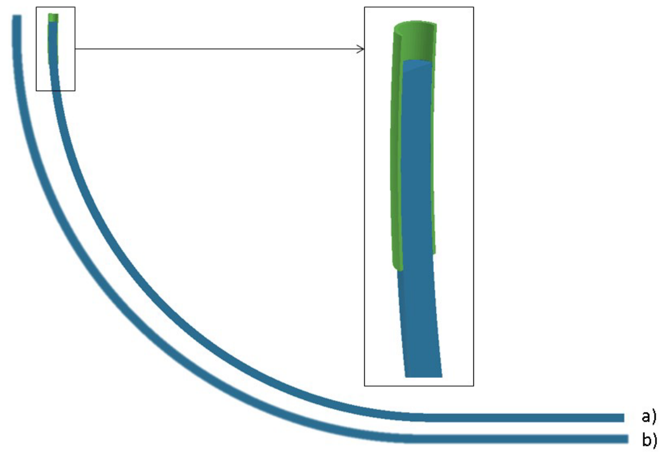


Fig. 2. The comparison of geometry of modelled area for computation under: a) Steady State Conditions, b) Traveling Boundary Conditions

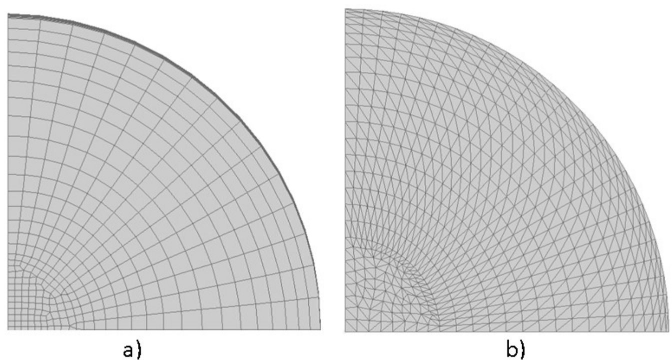


Fig. 3. The comparison of the computational mesh types for calculation of: a) temperature fields including the prediction of central porosity, b) stresses including the prediction of hot tears and cracks

4.3. Setting of Boundary Conditions

The Steady-State thermal calculation requires a definition of the inlet to the region. This inlet represents the surface of the steel in the mould. At the inlet, the constant casting temperature must be maintained. On the surface of the end of the casting strand, the adiabatic boundary condition was used. The water-cooling in the mould was defined by a heat flux boundary condition. The secondary cooling and the rolls were replaced with the thermal boundary condition. The casting speed and the strand movement were defined using the Solid Transport function.

In the case of the Traveling Boundary Condition, the initial casting temperature was applied to the whole volume of the modelled billet. The casting speed and the heat transfer along the casting strand were replaced by User Functions. The parameters and solver settings for the analysed test approaches are listed in Table 1 together with the casting temperature and casting speed

TABLE 1

Parameters and solver settings for the analysed test approaches

Approach	**Steady State Thermal Conditions with Solid Transport** Thermal and porosity calculation vs. Stress calculation	**Traveling Boundary Conditions** Thermal and porosity calculation vs. Stress calculation
Geometry	3D radial/straight with mould	3D radial/straight without mould
Computational domain	½ vs.1/4	½ vs. ¼
Mesh element type	Hexa and Wegde vs. Tetra	Hexa and Wegde vs. Tetra
Number of elements	475,300 vs.96,300	344,655 vs. 88,560
Initial time step size	0.001	0.001
Number of processors	4	4
Boundary Conditions		
Casting temperature [°C]	Temperature Inlet, T = const.	T = const. (whole geometry of modelled strand area)
Casting speed [m×s^{-1}]	Method of Solid Transport = 2 components of velocity defined by functions (vxsolidtransport.c and vysolidtransport.c)	v = const. (parameter used in User Functions of HF and HTC)
Mould Heat Flux	Water Cooling (Ambient Temperature + HTC)	User Function of HF (considering the gas gap formation)
Secondary Zone Cooling	Water Cooling: Ambient temp. + Emissivity + HTC Air Cooling: from database	User Function of HTC (including individual cooling subzones)
Operational Conditions		
Gravity [m×s^{-2}]	9.81	9.81

related with modelled steel grade; whereas Table 2 presents the more detailed values of selected defined boundary conditions. Also in the case of HF and HTC definition, it is necessary to adapt the intensity cooling according to the regime of casting.

TABLE 2

The detailed values of selected defined boundary conditions

Parameter	Value
Ambient temperature $_{\text{Air cooling}}$ [°C]	20
Heat Transfer Coefficient $_{\text{Air cooling}}$ [W×m^{-2}K^{-1}]	1000
Ambient temperature $_{\text{Water cooling}}$ [°C]	20
Heat Transfer Coefficient $_{\text{Water cooling}}$ [W×m^{-2}K^{-1}]	3000
Emissivity	0.85
Heat Flux $_{\text{Mould}}$ [MW×m^{-1}] from ref. [19]	3-1
Heat Transfer Coefficients $_{\text{Sec. Cooling}}$ [W×m^{-2}K^{-1}]	1400-270

5. Thermo-physical properties

It is obvious that both the thermo-physical, but also the stress properties of the steel significantly affect the quality of the numerical modelling results. In addition to the basic thermo-physical quantities, such as density, enthalpy, conductivity, or viscosity, attention should be paid also to the determined temperature of the steel liquidus and solidus, and therefore to the range of the two-phase zone.

Namely, the temperature of steel solidus (T_{Sol}) and liquidus (T_{Liq}) belong to the critical parameters particularly for casting and solidification of steel. Knowledge of precise T_L is important particularly for the setting of the temperature of steel superheating before its casting. The T_{Sol} is related in particular to the evolution of the solidification process as such, where conditions exist in the two-phase zone between the T_{Liq} and the T_{Sol}, which support a number of processes that may negatively influence the quality of the resultant solidified blank. The knowledge of these critical temperatures is important not only for the correct setting of the casting given by the technologies of casting and solidification of the steel intermediate products but also for an exact setting of the conditions of modelling of the evolution of the steel solidification. Correct setting of T_{Sol} together with T_{Liq} can then significantly influence also the results of numerical simulations, on the basis of which recommended interventions are made into the manufacturing technology in order to optimize the steel casting process.

It is assumed that experimental results with a high rate of reproducibility are more accurate than those that are calculated. In order to avoid a risk of jeopardy of steel production by the recommendation of suitable liquid temperatures, always the highest T_{Liq} is recommended for each grade/melt. The lowest T_{Sol} value obtained using thermal analysis methods is chosen as the T_{Sol} recommended for the industrial partner in accordance with the above approach.

5.1. Influence of the set thermo-physical properties of steel on the prediction of porosity

As mentioned above, continuous casting of steel is a rapid dynamic process of solid state change. The process of transition takes place within a certain temperature interval, which is referred to as a two-phase zone. The range of the two-phase zone is in the case of continuous casting of steel influenced not only by the chemical composition of the steel but also by the casting conditions. Higher casting speed usually results in longer metallurgical length, and in an extension of the two-phase zone. Extension of the metallurgical length and the length of the two-phase zone brings about an increased risk of the centerline porosity.

The sensitivity analysis of the calculation revealed that the determination of the thermo-physical parameters and namely of the temperatures of phase transformations is crucial for this calculation.

In the case of primary simulation, designated as variant A, the temperatures of phase transformation and thermo-physical properties of steel were determined by calculation in a thermodynamic database for a limited chemical composition, which, however, complied with the standard for the given steel grade. During the more precise specification of the model settings, the real chemical composition of the heat was then used for calculation of the thermo-physical properties and phase transformation temperatures. This model variant was designated as variant B. By specifying more precisely the chemical composition, which, however, in both cases fully complied with the standard for the given steel grade, namely the solidus temperature (T_{sol}) was modified, which dropped from the original value even by 20°C. Then, the two-phase zone (DT) represented 63°C above the original 44°C. The calculated temperatures of liquidus (T_{liq}), solidus and the range of two-phase zone of steel grade are listed in Table 3. The differences of the content of the elements of steel grade in wt.% are listed in Table 4.

The modelled variant B, which deferred in comparison with variant A only in a wider two-phase zone of modelled steel grade and in lower cooling intensity in final stage of secondary zone about 5%, led to a slight nuance in the stand shell thickness, which dropped from 22 to 21 mm in the area of the mould end, but to the extension of the metallurgical length about 11% (Fig. 4) and extension of the length of the two-phase zone up to 90%. All these changes in the final consequence resulted in an unequivocal detection of porosity (Fig. 4). The list of established qualitative parameters is given in Table 5.

TABLE 3

Temperature of liquidus, solidus and the range of two-phase zone of steel grade of the variant A and variant B

Variant	T_{liq} [°C]	T_{sol} [°C]	ΔT [°C]
A	1489	1445	44
B	1488	1425	63

TABLE 4

Differences in selected elements content of the chemical composition of the modelled steel grade between the variant A and variant B

Element	wt.% B – wt.% A
C	0.025
Mn	0.006
Si	0.013
P	0.0007
S	–0.0017
Cu	–0.0233
Ni	0.0067
Cr	0.0193
Al	–0.0157
Mo	0.0077

TABLE 5

The list of qualitative parameters obtained by numerical modelling

Parameter	Variant A	Variant B
Shell thickness [mm]	22	21
Metallurgical length [m]	14.7	16.3
Length of two-phase zone [cm]	168	319
The centerline porosity diameter [mm]	undetected	14

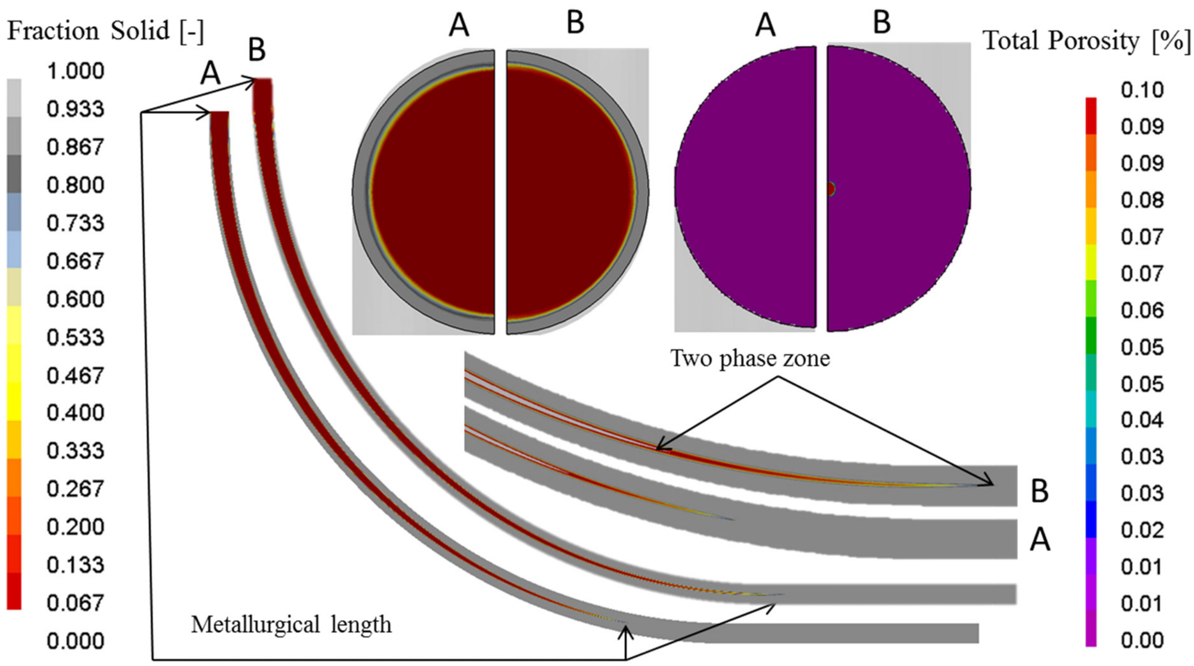


Fig. 4. The comparison of the qualitative parameters of modelled variant A and variant B

6. Conclusions

The paper presents the actual knowledge of the numerical modelling of solidification of continuously cast steel billets. The two approaches of modelling with finite element method used in ProCAST simulation software were described, namely the numerical modelling under the Steady State Thermal Conditions and the numerical modelling with the Traveling Boundary Conditions. It was found that:

- calculations allow the modelling of both straight and curved continuous casting processes;
- in the case of the Traveling Boundary Condition, the simplification of the geometry of the strand, which includes only the strand as such without mould, can be used;
- because of the calculation time, it is good also to reduce the number of mesh elements, for example by using only one symmetrical half of the geometry;
- in the case of the Steady State calculation, the boundary conditions, such as temperature inlet, heat flux, heat losses along the casting strand and the adiabatic condition at the end of the billet geometry, must be defined. The "movement" of the billet is described by the function Solid Transport, which defines the components of casting velocity in two directions in the case of the radial continuous casting machine;
- in the case of the Traveling Boundary Condition, the heat transfer along the casting strand is defined "only" with use of the User Function specified in programming language C++;
- the casting speed, casting temperature and the intensity of cooling were not the only significant parameters in the numerical model, a definition of thermo-physical properties also belonged to them;
- the correction of the two-phase zone of the modelled steel grade, which corresponded to the difference between the liquidus and solidus temperatures, led to an extension of the metallurgical length and also to the identification of porosity.

Based on these results, the next research will be focused on the verification of the numerical modelling not only under thermal condition, but also with considering of steel flow in the mould area and the submerged entry nozzle can be also included.

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