

A. BURBELKO*, J. FALKUS**, W. KAPTURKIEWICZ*, K. SOŁEK**, P. DROŹDŹ**, M. WRÓBEL*

MODELING OF THE GRAIN STRUCTURE FORMATION IN THE STEEL CONTINUOUS INGOT BY CAFE METHOD

MODELOWANIE KSZTAŁTOWANIA STRUKTURY WLEWKA COS METODĄ CAFE

Computer modeling of a temperature field and a solid phase fraction in casted billets is the base of any numerical simulation of the continuous casting technology. Temperature distribution in an ingot longitudinal and cross section for the same technological parameters is a function of solidification rate and rate of the solidification heat release. Nucleation rate and solid grain growth velocity depend on a melt undercooling below the liquidus temperature, and consequently depend on a temperature value. The results of the primary grain growth and temperature distribution modeling are presented for the square steel continuous casting 160×160 mm produced by CELSA Steel Works in Ostrowiec. For the modeling the ProCAST[®] software was used. Virtual structure of primary grains in the continuous ingot cross section was compared with a structure of a real ingot.

Keywords: ProCAST, structure, solidification, continuous casting, modeling

Podstawą modelowania matematycznego procesu ciągłego odlewania stali (COS) jest symulacja komputerowa pola temperatury i składu fazowego w obszarze wlewka. Rozkład temperatury wzdłuż wlewka i w jego przekroju przy zadanych parametrach odlewania zależy m.in. od intensywności przemiany fazowej, której towarzyszy wydzielanie się ciepła krystalizacji. Szybkości zarodkowania i wzrostu ziaren fazy stałej z ciekłej stali są uzależnione od jej przechłodzenia poniżej temperatury likwidus, a więc, w sposób pośredni od wartości temperatury. W pracy przedstawiono wyniki modelowania pola temperatury i procesu tworzenia się struktury pierwotnej stali B500 SP podczas krzepnięcia wlewka ciągłego o przekroju 160×160 mm, odlewane w warunkach CELSA HUTA OSTROWIEC. Do celów modelowania wykorzystano oprogramowanie ProCAST. Uzyskaną w symulacji strukturę ziaren pierwotnych w przekroju poprzecznym skonfrontowano z wynikami badań struktury rzeczywistej przekroju poprzecznego wlewków kwadratowych.

1. Mathematical modeling of the continuous casting solidification

In the earlier papers about the heat transfer in a continuous casting ingot the numerical solutions of the Fourier (or Fourier-Kirchhoff) partial differential equations were used [1-11]. For the numerical solution the Euler meshes were used. This kind of computational mesh is fixed in space. That is why additional calculations are needed to describe quantitatively the convective heat transport generated by the movement of an ingot solid part in a stationary coordinate system connected with an installation. The phenomena of the grain nucleation and growth in the aforementioned publications are not taken into account.

The attempts of the microstructure formation modeling in the continuous casting as results of the grains nucleation and growth are shown in [12, 13]. The so-called *micro-macro* model was used in these papers. In the *micro-macro* modeling the heat transfer process was analyzed in scale of an ingot (*macro*). Mathematical model of the nucleation and growth of solid grains in the *micro-scale* make it possible to predict the structure formation and calculate the rate of the solidification latent heat release. The main disadvantage of such kind of models is the assumption of the equiaxed crystal shape. In the *micro-macro* modeling the mean statistical values of parameters (for example mean grain size or grain density) are used for the structure characterization. It is not possible to predict the depth of the columnar structure

* AGH UNIVERSITY OF SCIENCE AND TECHNOLOGY, FACULTY OF FOUNDRY ENGINEERING, 30-059 KRAKÓW, 30 MICKIEWICZA AV., POLAND

** AGH UNIVERSITY OF SCIENCE AND TECHNOLOGY, DEPARTMENT OF FERROUS METALLURGY, FACULTY OF METALS ENGINEERING AND INDUSTRIAL COMPUTER SCIENCE, 30-059 KRAKÓW, 30 MICKIEWICZA AV., POLAND

zone or the relation between the longitudinal and lateral sizes of columnar grains.

Modeling of the inner structure of the dendritic grain by means of the cellular automaton (CA) method in two dimensions is presented in [14]. Modeling of the thin segregation layer formation under a small freezing crystals layer in a continuous strand is shown in [15]. Unfortunately, CA models with a cell size of order of $1\ \mu\text{m}$ cannot be used for the solidification modeling on a large scale typical for industrial continuous casters.

In this paper the CAFE model [16-17] is available as ProCAST[®] software module [18] was used for the simulation of a primary phase grains in a continuous ingot. In this modeling Cellular Automata (CA) mathematical method is used with a greater cell size sufficient for outer grain shape modeling. The CA modeling enables to take into account the stochastic bulk and surface (at the crystallizer wall) grain nucleation, as for simulating individual growth of the primary phase grains. Results of simulation are history of the interphase boundary migration as well as the grain boundary position after the full ingot solidification. A CA simulation is connected with an ingot temperature field calculation. For heat flux and temperature field modeling the Finite Element Method (FEM) was used in the ProCAST[®] software. As opposed to the model [14] mentioned above, the CAFE model works with the cell size of order 0.1 mm, that is why the simulation of an inner structure of dendritic grains is not possible. On the other hand the three-dimensional analysis of greater domains is able to work in CAFE.

The CA modeling of the microstructure formation during the continuous ingot solidification requires the mobile Lagrange's mesh utilization connected with an ingot.

2. Conditions of modeling

The calculations were performed for the square ingot of the section $160 \times 160\ \text{mm}$ produced by CELSA Steel Works Ostrowiec (CELSA Group). The curvature of the continuous ingots is constant from the crystallizer up to the straightening machine and the radius of the inner ingot surface is equal to 10 m. Due to the appropriate shape of the crystallizer's walls the bending of an ingot in this continuous caster is not necessary.

For the ingot temperature field calculation the Lagrange's mesh was used connected with the ingot. The domain of the casting used in the simulation is divided into 3 sub-domains as it is shown in Fig. 1. The sub-domain 2 in this figure is used for the intrinsic ingot temperature representation and the solidification path modeling. The sub-domains 1 and 3 are used as buffer zones: the upper sub-domain (1) is used for the emula-

tion of heat influence of the up-stream ingot part on the main sub-domain (2), and the lower sub-domain (3) – for the emulation of down-stream part influence.

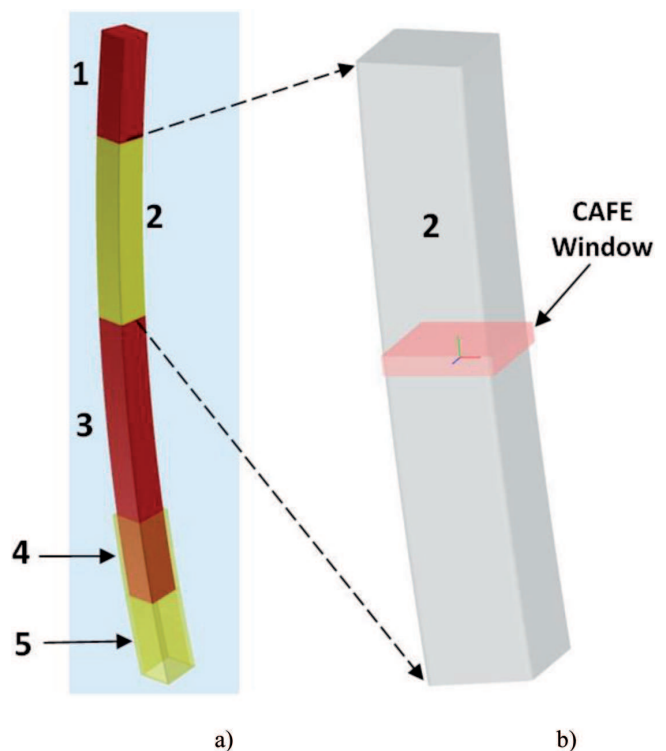


Fig. 1. Scheme of the sub-domains geometry in the simulation domain: a) calculation sub-domains in the crystallizer and ingot; b) CAFE sub-domain (2) with a CAFE window

The equal curvature of the ingot and crystallizer adjoining surfaces give the possibility of using Lagrange's mesh for the temperature calculation in the crystallizer. The FEM mesh in the crystallizer is connected with its body and during the solution calculations it has rotary axis motion relative to the curvature axes (common for the crystallizer and an ingot). The examples of the crystallizer positions in the background of the ingot temperature field are shown in Fig. 2 (the crystallizer is transparent). The crystallizer's height is equal to 900 mm. The crystallizer's domain is divided into two sub-domains (4 and 5 in Fig. 1). Border position of these sub-domains is connected with the liquid steel level in the crystallizer and the meniscus' position. Lower sub-domain (5) is in thermal contact with steel (see Table 1). Upper sub-domain (4) is isolated from the ingot sub-domains. The uniform initial temperature distribution was assumed for the ingot and the crystallizer. That is why the ingot upper sub-domain (3 in Fig. 1) has the additional function – stabilization of temperature distribution and heat flux in the crystallizer.

The length of the cooling zones in the continuous casting machine used in the modeling and adopted heat transfer coefficients are shown in the Table 1.

TABLE 1

Conditions of the ingot cooling

	Discharge of water, l/min. (min / max)	Sub-domain length, m	Mean specific discharge of water, l/(min. · running meter)	Heat transfer coefficient, W/(m ² · K)
Crystallizer		0.60		1000
Sub-domain I	196 / 220	0.50	397	550
Sub-domain II	276 / 335	2.72	95.0	400
Sub-domain III	136 / 163	2.93	51.0	300
Sub-domain IV	76 / 90	3.19	26.0	200

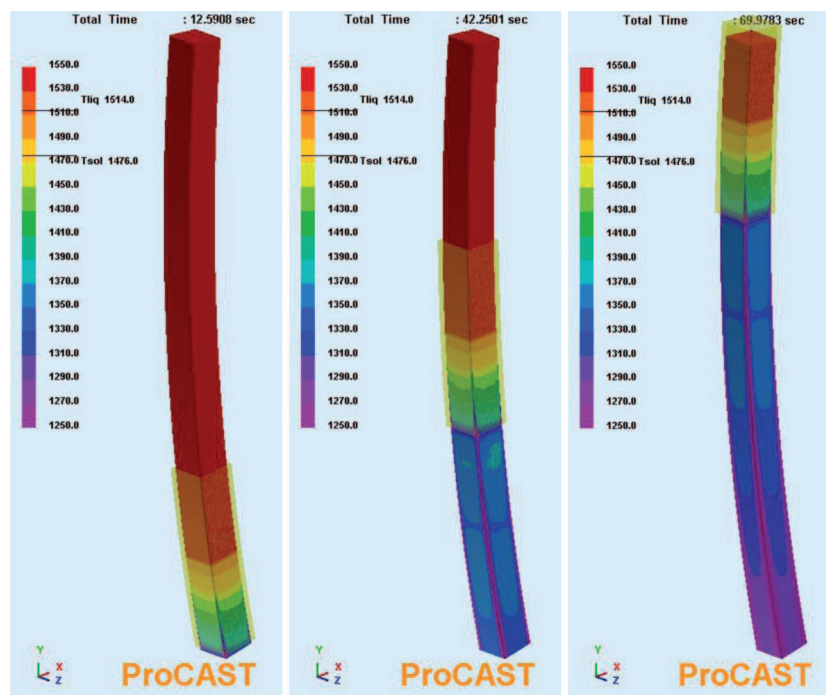


Fig. 2. Relative crystallizer and continuous ingot movement: transparent crystallizer on the background of the casting temperature field

Simulations were performed for two steel grades: B500 SP and S235JR. The chemical compositions of the steels used in the modeling are shown in the Table 2. The materials' parameters for the calculation were estimated by the module of the thermodynamic database CompuTherm (CompuTherm, LLC [19]) built-in into the ProCAST software. Temperature dependence of the heat conductivity, density and enthalpy as well as solidification path of these steels are shown in Fig. 3. It should be noted that the used version of this module does not take into account the possibility of MnS precipitation. Sulfides solidification gives lower solidus temperature. The comparison of the enthalpy tempera-

ture dependence for the analyzed steels used in the modeling and obtained by the Thermo-Calc software based on the Calphad Method [20] is shown in Fig. 3d.

Grain nucleation on a crystallizer's surface as well as in an ingot bulk has a heterogenic nature with a stochastic nucleation distribution in the space. The number of active substrates for nucleation is the function of undercooling. These values are connected by the Gauss (normal) statistical distribution function with the mean value ΔT_m and the standard deviation ΔT_σ [21]. The values of surface and bulk substrates densities as well as Gauss function parameters used in the modeling are shown in Table 3.

TABLE 2

The chemical compositions of the steels used in the modeling (weight percent)

Steel grade	C	Mn	Si	P	S	Cu	Cr	Ni	Mo	Al
B500 SP	0.208	0.863	0.153	0.027	0.034	0.3	0.102	0.098	0.021	0.004
S235JR	0.13	0.53	0.16	0.018	0.015	0.3	0.09	0.09	0.02	0.004

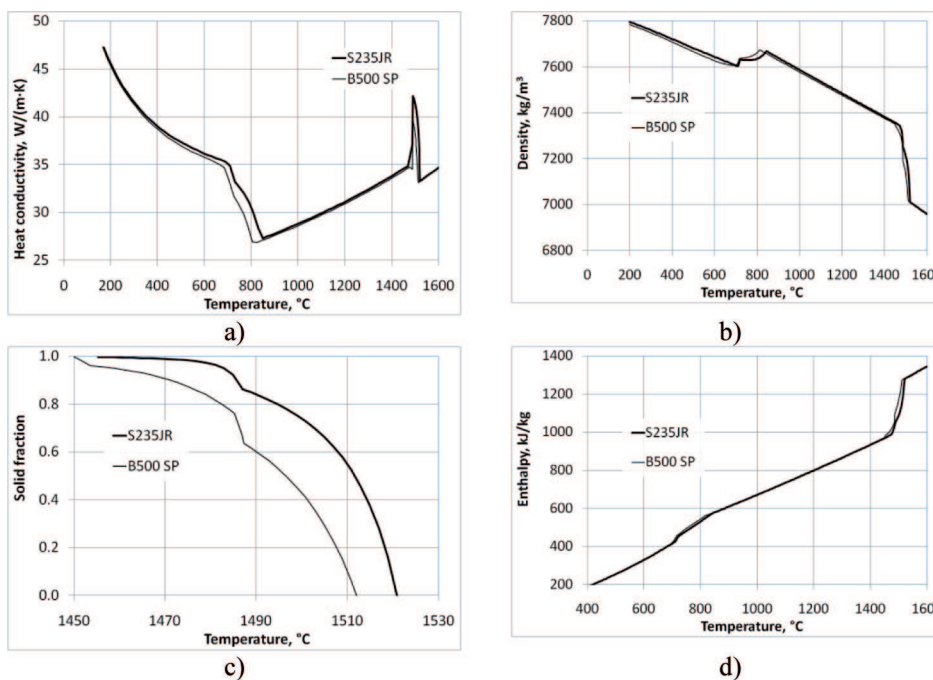


Fig. 3. Temperature dependence of the heat conductivity (a), density (b), solid fraction (c) and enthalpy used in the simulation

TABLE 3

Nucleation law parameters used in the modeling

Type of nucleation	Substrates density	ΔT_m	ΔT_σ
bulk	$1.0 \cdot 10^8 \text{ m}^{-3}$	30	10
surface	$5.0 \cdot 10^6 \text{ m}^{-2}$	15	5

3. Results of the simulations

The modeling of the primary grain growth and microstructure formation was performed only in the CAFE Windows (see Fig. 1). The calculated cooling curves for the three points placed in the *CAFE Window* at the ingot centerline, at the center of lateral wall and on the ingot edge are shown in the Fig. 4. Local temperature growth in the outer points (at the ingot’s wall and edge) takes place in the moment when ingot cross-section pass from one cooling zone to another with a lower specific discharge of water. In the modeling this is taken into account by means of the different heat transfer coefficient values (see Table 1). As it is shown in the Fig. 4, the metallurgical length of the S235JR strand obtained by

modeling is equal to 20.6 m. This value is 1.0 m shorter than metallurgical length obtained for B500 SP steel grade. This difference may be explained first of all by the difference in the solidus temperature of the analyzed steels (see Fig. 3c).

The results of the primary grain structure obtained in the modeling by the cellular automaton method in the longitudinal and cross section are shown in Fig. 5. Near the ingot surface the narrow zone of small equiaxed chilled grains is visible. In the centerline area big equiaxed grains are not observed. In fact the ingots have the columnar structure in almost whole cross section (except the thin equiaxed chilled surface layer). The similar structure is observed in the real continuous castings. The results of the real ingot cross section structure examina-

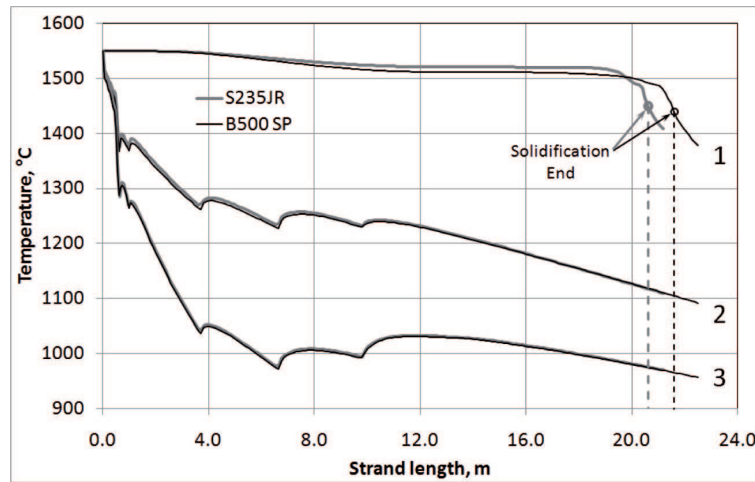


Fig. 4. Temperature distribution along the continuous ingot: at the ingot middle line (1), at the middle of lateral surface (2) and on the edge (3) – the results of the simulation

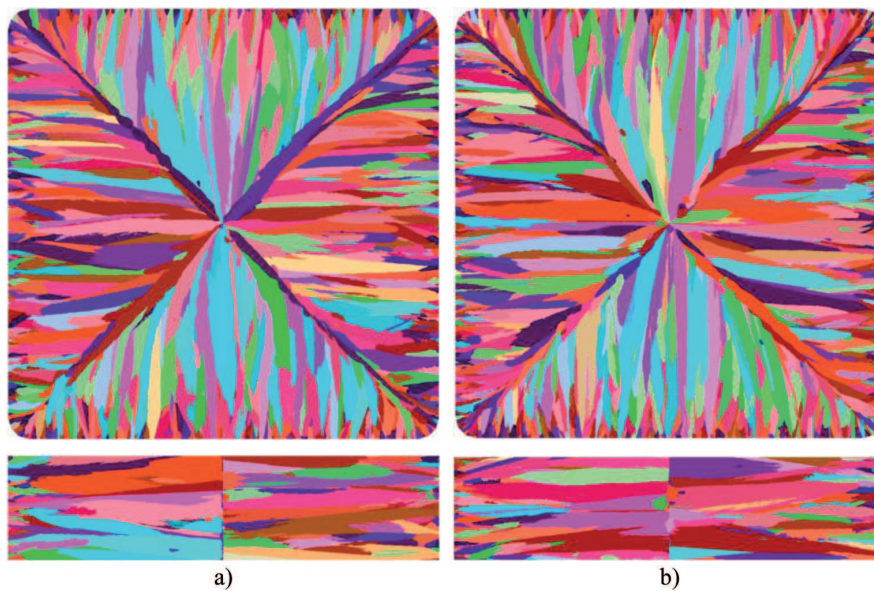


Fig. 5. Primary grains' structure of the S235JR (a) and B500 SP (b) steel in the cross and longitudinal sections of the continuous strands of size 160×160 mm (modeling)

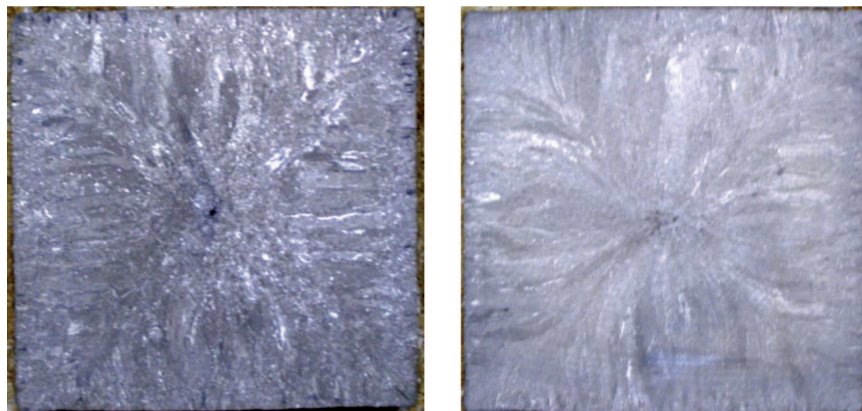


Fig. 6. The samples of the cross section structure in the continuous ingot of size 160×160 mm. Steel grade S235JR (PN-EN 125-2)

tion are shown in the Fig. 6. These results are obtained for the quadratic continuous ingot of size 160×160 mm manufactured by CELSA HUTA OSTROWIEC from the steel S235JR (PN-EN 125-2).

Comparison of the Fig. 5 and 6 indicates that results of the continuous ingot structure modeling by means of the CAFE method gives a good representation of microstructure of product.

4. Conclusions

The CAFE module of the ProCAST software is a useful tool for the modeling of the primary structure formation in a continuous ingot.

In the modeling of quadratic ingots of size 160×160 mm the obtained structure includes the narrow zone of small equiaxed chilled grains near the surface and the wide zone of columnar grains. The similar structure was obtained in the practical examination of a commercial continuous ingot with the 160×160 mm cross section. The zone of equiaxed grains near the ingot middle line is not observed as in the modeling as in the practical examination of these ingots.

Acknowledgements

Research work was supported by the European Regional Development Fund – the Operational Programme – Innovative Economy, as a project “New Concept for Selection of the Cooling Parameters in Continuous Casting of Steel”, POIG.01.03.01-12-009/09.

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