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Prediction of Dendritic Microstructure Using the Cellular Automaton – Finite Element Method for Hypoeutectic Al-Si Alloys Castings

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In the present paper the description of Al-Si alloy structure modeling using the Cellular Automaton – Finite Element method was briefly presented. This method was adopted to predict the pseudo-dendritic grain microstructure arising during solidification process of castings. Testing of this casting was connected with an attempt of validation of the Calcosoft System (CS-CAFE). Applications are given for prediction of grains size, columnar-to-equiaxed transition (CET) zones for hypoeutectic Al-Si alloys for cylindrical castings which solidify in homogeneous mould and also in moulds containing the chill. Validation has been carried out using a simulation-experiment method under various conditions of thermal interaction between the casting and mould. The results of metallographic studies of experimental casting structure have been adjusted to CAFE prognosis, i.e. simulation structure.
Keywords: castings, Al-Si alloy, micromodelling, prediction of microstructure.

1. INTRODUCTION

Crystalline structure of castings consists mostly of dendritic columnar and equiaxed crystals. The kind of resulting crystals depends on the concentration of admixture component in the alloy and on the undercooling of liquid phase before crystallization front. Modeling of the structure was developed on the basis of deterministic models describing nucleation and growth of equiaxed crystals. The models contain considerable simplification and limitations [1]. For these reasons models based on stochastic methods were introduced.

In the first place modeling using the Monte Carlo method was developed [2]. In this method the mechanism of crystal growth does not adequately reflect the physical process. In 1992 so-called cellular automaton started to be used [3]. The method consists of prediscretization of the casting by means of finite elements – FE (thermal model) and secondary meshing of the space (modeling of crystal nucleation and growth with use of Cellular Automaton – CA). This model is here referred to as CAFE. Initially the two-dimensional models (2D) were worked out, next they were developed into the 3D model.

In this paper our first research on the full CAFE-3D model of the Calcosoft system is described.

2. DESCRIPTION OF THE CAFE – 3D MODEL

In the simulation research described below the Calcosoft 3D system was applied with the module CAFE [4], used for modeling structures of castings, in which columnar and equiaxed crystals are formed. The model is based on combination of calculation of heat transfer by means of finite elements method with calculation using the principle of cellular automaton describing the process of crystal nucleation and growth.

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This model assumes that crystal nucleation takes place on the surface of the mould and in the bulk of liquid alloy according to two curves of nucleation intensity, which are activated in the function of undercooling. M. Rappaz [5] proposed Gaussian distribution for the description of nucleation intensity $dn/d(\Delta T)$, to determine in this way the local density of crystals (grains). The distribution $dn/d(\Delta T)$ is described by the equation

$$\frac{dn}{d(\Delta T)} = \frac{n_{max}}{\sigma_{\Delta T} \cdot \sqrt{2\pi}} exp\left[-\frac{1}{2}\left(\frac{\Delta T - \Delta T_m}{\sigma_{\Delta T}} \right)^2 \right] \quad (1)$$

where: ΔT is the calculated local undercooling, ΔT_m is the mean undercooling, $\sigma_{\Delta T}$ is the standard deviation, n_{max} is the maximum nucleation density which can be reached when all the nucleation sites are activated while cooling (n_{max} is determined experimentally with the given alloy).

At the beginning of the calculation, nucleation sites are distributed in the cells of the defined CA mesh (Fig. 1). The number of nucleation sites N^{nuc} is attributed to CA cells randomly chosen from the given volume V and is described as $N^{nuc} = n_{max} \cdot V$. For each nucleation cell marked as ν and chosen at random, the nucleation undercooling $\Delta T_\nu^{nuc} = T_L - T_\nu^{nuc}$ (where T_L is the liquidus temperature, T_ν^{nuc} is the critical nucleation temperature) is also randomly attributed according to Gaussian distribution. The CAFE-3D algorithm uses a dynamic allocation of the cells (Fig. 1). Initialization of nucleation algorithm is repeated every time when new liquid cells are dynamically allocated during the CA calculation. At the beginning of calculation the temperature of the alloy is higher than the liquidus temperature. All the cells are respectively marked by state index $i = 0$ (liquid state). New crystals are formed as the result of the fall of local temperature of nucleating cell below the critical temperature T_ν^{nuc} in the given time step $\delta t \le \delta t_{max}$ (where: $\delta t_{max} = l_{cell}/\upsilon_{\Delta T max}$, l_{cell} – length of the CA mesh, $\upsilon_{\Delta T max}$ – velocity of dendrite tip growth at maximum undercooling ΔT_{max}). In this case the index is

changed into integer corresponding to the crystal index *(i ≠ 0)*. Crystalographic orientation of crystal growth is randomly chosen from among predefined orientation classes. At the beginning of calculation crystal growth orientation classes are initiated through randomly selected three Euler angles *(Φ_1, Φ, Φ_2)* defining rectangular distribution of directions <100> [6].

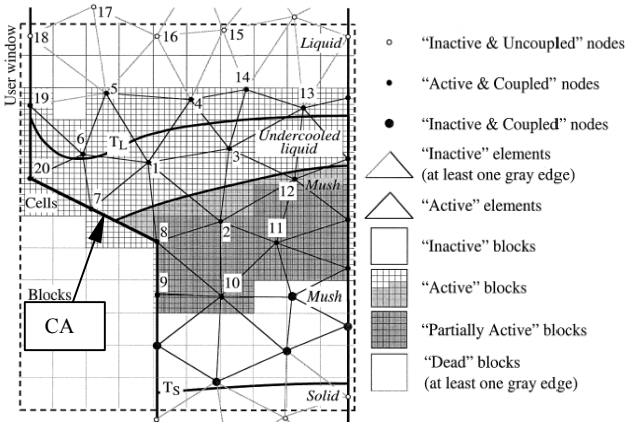

Fig. 1. Scheme of dynamic allocation of defined windows, blocks and cells in case of full coupled of calculation in CAFE-3D model [5]

The crystal growth is based on octahedron bounded by faces [111]. To each growing cell there is ascribed an index of total value *($i_\nu \neq 0$)*. During calculation at least one of the neighboring cells CA is in liquid state. The growing octahedron associated with the cell – ν *($i_\nu \neq 0$)* „capturing" the cell center of one of the neighboring cells – μ ($i_\mu = 0$) is shown in Fig. 2. The state index of the „captured" cell μ is changed into those of the ν cell. The growth of a new octahedron associated with the cell μ will not proceed when the cell is fully surrounded by mushy cells. The main diagonals of the octahedron (referred to the axis *X*, *Y*, *Z*) correspond to the crystallographic orientation <100> along which dendrite arms develop. The directions are defined by Euler angles.

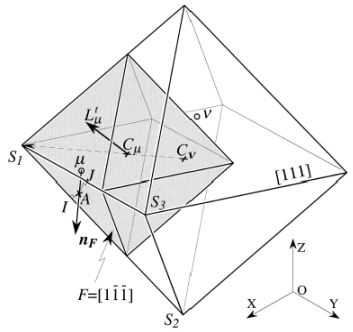

Fig. 2. Schematics of the decentered octahedron CA growth algorithm [5]

Calculation of kinetics of the dendrite tip growth $\upsilon_{\Delta T}$ is done according to the model of Kurz et al. [7]. The ν cell increment along trunk diagonals of the associated octahedron is given by equation [5]:

$$\Delta R_\nu = \upsilon_{\Delta T_\nu} \cdot \delta t \ , \qquad (2)$$

where: $\upsilon_{\Delta T_\nu} = a_2 \cdot \Delta T^2 + a_3 \cdot \Delta T^3$ – empirical dependence on the velocity of the dendrite tip growth for the calculated undercooling ΔT in the cell ν.

3. INVESTIGATION OF THE SELECTED PARAMETERS OF STRUCTURE OF THE SILUMIN CASTING

Experimental tests have been carried out on cylindrical castings of 70 mm diameter and 220 mm height made of unmodified AlSi7 alloy. The castings were made in the mould shown in Fig. 3. Three combinations of materials for the mould were used: silica moulding sand (Q-Q), silica moulding sand and copper chill (Q-Ch), high insulating sand and copper chill (Hi-Ch). Parameters of the structure obtained (only dendrites of α solid solution) have been described, considering the position of transition zone of columnar-to-equiaxed CET crystals and the size of equiaxed crystals.

Simulation studies carried out with the use of Calcosoft 3D system with the CAFE module have been preceded by identification and determination of physical conditions of the experiment.

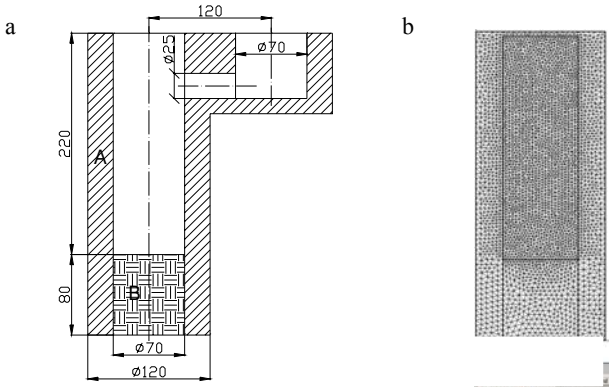

Fig. 3. Scheme of mould: a – experimental, b – virtual

The following values of physical parameters have been adopted for the simulation:

constant value parameters:

– characteristic temperatures were determined on the ground of experimental cooling curves of casting: initial temperature of alloy in the mould 700 °C, liquidus T_L = 602 °C, eutectic T_e = 574 °C, solidus T_{sol} = 572 °C, initial of mould and external 20 °C;

– latent heat 419 000 J/kg;

– heat capacity, kJ/(m^3·K): of the alloy in liquid phase $C^{'}$ = 3483, in solid phase C = 2700; of silica sand C_Q = 1500, of insulating material C_{Hi} = 587, chill C_{Ch} = 3300,

– heat transfer coefficient, W/(m^2·K): casting-mould $\alpha_{cast\text{-}m} = 10^4$, $\alpha_{ambient}$ = 20,

– thermal conductivity, W/(m·K) liquid λ_L = 90 and solid phase λ_S = 130,

and postulated parameters for empirical relations:

– undercooling of alloy, °C: on a surface of the homogenous mould ΔT_{ms} = 5,

– standard deviation, °C: $\sigma_{\Delta T}$ = 0.4,

– grow kinetic coefficient a_2 , ms^{-1}K^{-2}: 2.9·10^{-6};

variable value parameters:

– thermal conductivity of mould, W/(m·K): silica sand $\lambda_Q = 0.5 \div 1.5$, microsphere (high insulation) $\lambda_{Hi} = 0.15 \div 0.5$,

– heat transfer coefficient, W/(m^2·K): casting-chill $\alpha_{cast\text{-}Ch} = 100 \div 8000$,

and postulated parameters for empirical relations:

- maximal density of nuclei, m^{-2}, m^{-3}: silica sand mould: n_s (at the mould surface) $=10^4 \div 10^7$, n_v (in the bulk of liquid) $= 10^5 \div 10^9$, mould with chill: n_s (at the mould surface) $= 10^5 \div 10^6$, n_{Ch} (at the chill surface) $= 5\cdot10^5 \div 5\cdot10^6$; $n_v = 10^5 \div 10^8$,

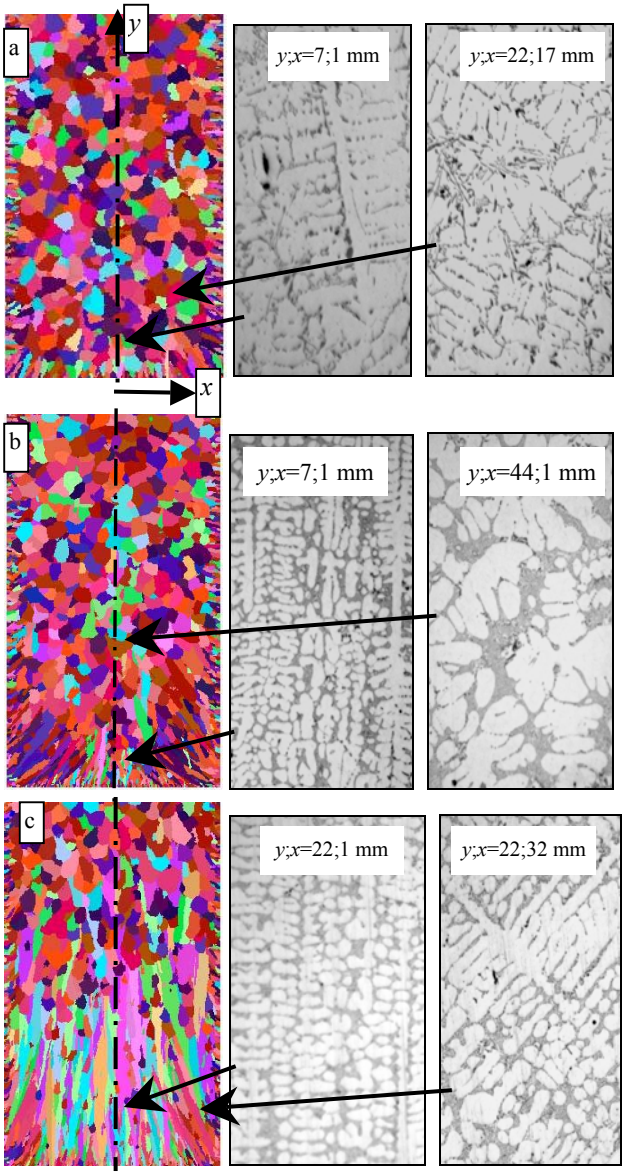

Fig. 4. Virtual and experimental structure solidify in mould: a – silica sand (ΔT_{ms}=2 °C, ΔT_{mv}=5 °C, $\sigma_{\Delta Tv}$,$\sigma_{\Delta Ts}$ = 0.4 °C, $n_s = 10^6$ m^{-2}, $n_v = 10^7$ m^{-3}, $\lambda = 0.75$ W/(m·K), $\alpha_{cast\text{-}m}$ = $=10^4$ W/(m^2·K), a_3=1.49·10^{-6} m/(s·K^3)); b – silica sand with chill (ΔT_{ms}=5 °C, ΔT_{mCh}=15 °C, ΔT_{mv}=4 °C, $\sigma_{\Delta Tv}$,$\sigma_{\Delta Ts}$ and $\sigma_{\Delta TCh}$=0.4 °C, $n_s=10^6$ m^{-2}, $n_{Ch}=5\cdot10^6$ m^{-2}, $n_v=10^7$ m^{-3}, $\lambda = 0.75$ W/(m·K), $\alpha_{cast\text{-}Ch} = 800$ W/(m^2·K), $a_3 = 3\cdot10^{-8}$ m/(s·K^3)); c – insulation sand with chill ($\Delta T_{ms} = 5$ °C, $\Delta T_{mCh} = 15$ °C, $\Delta T_{mv} = 4$ °C, $\sigma_{\Delta Tv}$,$\sigma_{\Delta Ts}$ and $\sigma_{\Delta TCh} = 0.4$ °C, $n_s = 10^6$ m^{-2}, $n_{Ch} = 5\cdot10^6$ m^{-2}, $n_s = 10^7$ m^{-3}, $\lambda = 0.5$ W/(m·K), $\alpha_{cast\text{-}Ch} = 4000$ W/(m^2·K), $a_3 = 3\cdot10^{-8}$ m/(s·K^3))

- undercooling of the alloy, °C: homogenous silica sand mould: in the bulk of liquid ΔT_{mv}=1÷10, mould with chill: at the surface $\Delta T_{ms} = 1 \div 8$, ΔT_{mCh} (at the chill) = $= 2 \div 15$, $\Delta T_{mv} = 1 \div 15$,

– grow kinetic coefficient a_3, ms^{-1}K^{-3}: silica sand mould: $10^{-8} \div 10^{-6}$, silica sand mould with chill: $1.5\cdot10^{-8} \div 1.5\cdot10^{-6}$.

The results of simulation study of the castings solidifying in the defined moulds in the forms of virtual structures (shape, size and position of the CET zone) obtained from the calculations are illustrated in Fig. 4 for the cases of best conformity with the actual structure. The values of the simulation parameters are presented under Fig. 4. The location of the CET zone and the size of equiaxed crystals is given in Table 1. There is also there the deviation of simulation results and of the experiment with CET in terms of percentage ($\Delta_{CET} = (CET_S - CET_E)100\,/CET_E$, in %) and the mean diameter of equiaxed crystals – d ($\Delta_d = (d_S - d_E)100/d_E$, in %), where the indices are: S – result of the simulation, E – the result of the experiment. For the castings made in silica sand (Q-Q) moulds and silica sand mould with chill (Q-Ch) the relative differences Δ_{CET} and Δ_d are about 20 %. In the insulating mould with chill (Hi-Ch) Δ_d is about 20 %, and Δ_{CET} = 3.6 %.

Table 1. CET distance and equiaxed grains size taken from simulation (S) and experiment (E)

Casting mould		CET mm	Mean diameter of equiaxed grains d, mm		
			distance from bottom, mm		
			15	35	70
Q-Q	*S*	6	3.1	3.5	3.7
	E	5	3.7	4.4	4.9
	Δ, %	20	–16.2	–20.4	–24.1
Q-Ch	*S*	17	–	3.0	3.5
	E	14	–	3.6	4.4
	Δ, %	21	–	–16.7	–20.4
Hi-Ch	*S*	60	–	–	2.9
	E	62	–	–	4.3
	Δ, %	3.2	–	–	–23.6

The small value of Δ_{CET} is the result of good adjustment of parameters used in simulation for the casting solidyfing directionally (high values CET).

The analysis and selection of thermophysical coefficients and the postulated parameters in the empirical interrelations required for the simulation in order to obtain good conformity of the crystalline structure with the experiment are easier when their impact on the virtual structure is known. The results of the study of the influence of those parameter values in the CAFE model on CET are shown in Fig. 5 for the castings solidyfing in the condition of a homogenous silica sand mould (Q-Q) and in Fig. 6 for the mould with the chill (Q-Ch).

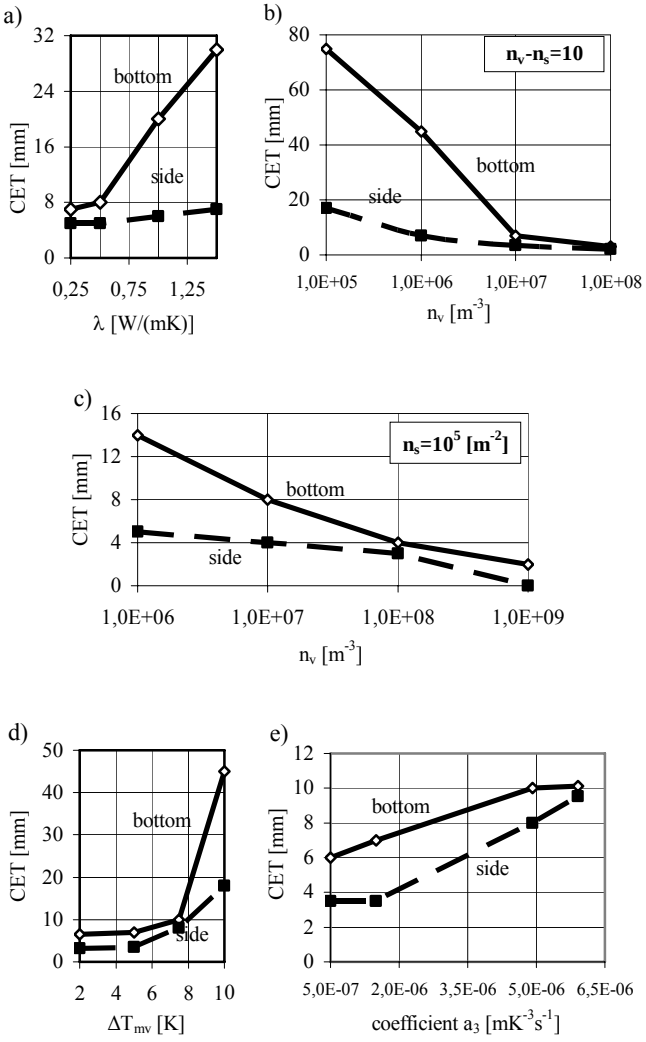

Fig. 5. CET relationship in silica sand mould casting from: a – λ of moulding sand; b, c – number of nuclei in the bulk of liquid, d – mean undercooling in a bulk of liquid, e – a_3 coefficient; at the constance value of rest parameters: ΔT_{ms}=2 °C, ΔT_{mv}=5 °C, $\sigma_{\Delta Ts}$, and $\sigma_{\Delta Tv}$=0.4 °C, n_s=10^6 m^{-2}, n_v= 10^7 m^{-3}, λ = 0.5 W/(m·K), $\alpha_{cast\text{-}m}$ = 10^4 W/(m^2·K), a_3 = 1.49·10^{-7} m/(sK^3)

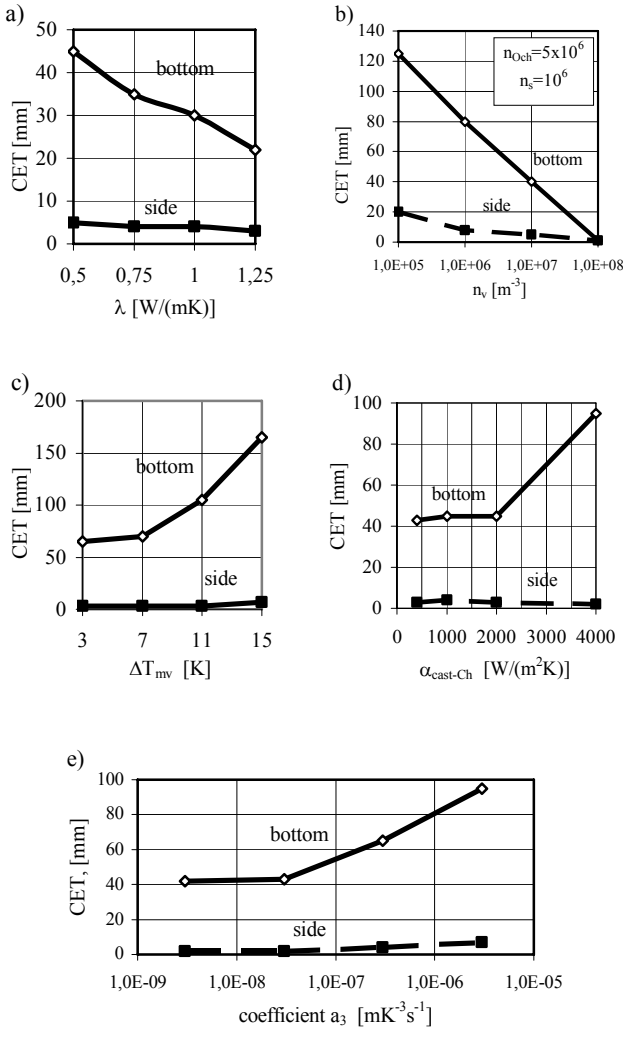

Fig. 6. CET relationship in silica sand mould with chill casting from: a – λ of moulding sand; b, c – number of nuclei in the bulk of liquid; d – mean undercooling in a bulk of liquid, e – a_3 coefficient; at the constance value of rest parameters: ΔT_{ms} = 5°C, ΔT_{mCh} = 15°C, ΔT_{mv} = 4°C, $\sigma_{\Delta Tv}$, $\sigma_{\Delta Ts}$, $\sigma_{\Delta TCh}$=0.4°C, n_s=10^6 m^{-2}, n_{Ch}=5·10^6 m^{-2}, n_v=10^7 m^{-3}, λ=1.0 W/(m·K), $\alpha_{cast\text{-}Ch}$=800 W/(m^2·K), a_3=3·10^{-8} m/(s·K^3)

From the presented graphs it follows that within the examined range the intensity of influence of the growth of the CET value is bigger when the number of nuclei in the volume in the case of a sand mould $n_v < 10^7$ (with $n_v - n_s = 10$), the mean undercooling of the alloy in the volume $\Delta T_{mv} > 8$ °C (with $\sigma_{\Delta T} = 0.4$ °C) and coefficient $a_3 = 2 \cdot 10^{-7} \div 5 \cdot 10^{-6}$ (sand mould) and $a_3 > 5 \cdot 10^{-8}$ (mould with chill). The increment of λ_{mould} of homogenous mould causes the increment of CET, higher when $\lambda_{mould} > 0.5$ W/(mK)). The tendency of λ_{mould} influence on CET in the mould on the side of the chill in the (Hi-Ch) mould is contrary to that in the homogenous (Q-Q) mould. The values of the simulation parameters have greater influence on CET on the side of base of the cylinder than from the surface of the cylinder.

CONCLUSIONS

1. The Calcosoft 3D system with CAFE module needs special validation to obtain the satisfying conformity with the results of the experiment in relation to the location of CET zones and the size of equiaxed crystals in test castings solidyfing in homogenous moulds and made of materials diversified in thermal aspect.
2. The testing and analyzing of the influence of the value of thermophysical coefficients and parameters indispensable to complete the empirical interrelations used for simulation of crystalline structure formation presented in this paper is useful. Without this validation the application of the CAFE module is merely of cognitive character and not that expected – utilitarian.

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