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Sensitivity testing practice on pre-processing parameters in hard and soft coupled modeling

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Abstract

This paper pays attention to the problem of practical applicability of coupled modeling with the use of hard and soft models types and necessity of adapted to that models data base possession. The data base tests results for cylindrical 30 mm diameter casting made of AlSi7Mg alloy were presented. In simulation tests that were applied the Calcosoft system with CAFE (Cellular Automaton Finite Element) module. This module which belongs to „multiphysics" models enables structure prediction of complete casting with division of columnar and equiaxed crystals zones of α-phase. Sensitivity tests of coupled model on the particular values parameters changing were made. On these basis it was determined the relations of CET (columnar-to-equaiaxed transition) zone position influence. The example of virtual structure validation based on real structure with CET zone location and grain size was shown.

Keywords: Multiphysics, Multiscale, Structure modeling, Solidification, Cellular automata

1. Introduction

Structure zones are the specific feature of each casting. There is well-known literature example of ingot scheme which structure consists of outer grains, columnar and equiaxed grains. That is known that dendritic character of grains (crystals) in each of these zones considers single-phase alloy. The boundaries of these zones are very accurate. That assumption about structure zones display was made because of didactic point of view. The previous papers published also by our team [1,2,3] shown that real zones transition of handbooks' casts structures even in intensive chill conditions there are not simple to identify. Especially when there are taken into consideration multi-phase alloys. Additionally the prediction of quantity and kind of phases which is based on the phase diagrams should often be modified because of crystallization conditions of thermodynamic equilibrium deviation. It also considers the structure defects in micro and macro scale (shrinkage, other types of discontinuities, degenerate phases, phases being the effect of macro/microsegregation, non-metallic inclusions). Their location is very difficult to formulate in so-called hard modeling of phenomena. This is the reason why that is important to implement the empirical knowledge [4,5,6] rather adjusted to theoretical basis.

Casting structure differentiation should be skillfully utilized from part design through technology design stage to virtual prediction and quality control of final castings using NDT methods, it was described in [7].

Nowadays there is formal possibility of structure prediction using simulation systems basing on coupled modeling of hard and soft models. Hard models (i.e. these kinds which are based on physical laws and differential equation) disable satisfactory formulation of so complex phenomenon like crystallization process. This is the reason why it is still important to search the effective solutions in Multiscale and Multiphysics area [8,9]. These systems formulate the various phenomena coupling in one coupled model taking into account discrete meshing (macro-micro). The purpose is the test of the best comprehensive fitting to real process. However there are new validation tasks which have to be undertaken parallel with models creation which are expected to be coupled. Introducing the soft models is expected to be indispensable in order to find the solution of "multiscale" modeling problem useful in foundry industry [10]. In [8] it was shown lots of interesting generalized suggestions related with this problem.

Relatively good tool to selected parameters of casting structure prediction concerning its local differentiation is Calcosoft CAFE system [11,12,13]. The prediction depends on forecast structure formation of blocs shape (crystallites) at different refinement and also their spatial orientation. However CAFE model has certain limitation. It concerns the prediction of α - phase formation applying to hypoeutectic Al-Si alloys while the eutectic phase is neglected. Deducing about α - phase location in virtual map structure has to be referred to real structure and to zones of the virtual crystallites boundaries. For that kind of hypoeutectic alloy the model was elaborated and described in [11,12] while in [13,14] it was made the authentication of validation basis of applied coupled model.

The modeling scales can be formally divided into four groups [15] which refer to four simulation (modeling) systems generation. It formulates the phenomena of crystallization and solidification of castings: macro, mezzo, micro, nano.
Unfortunately the majority of described models from Multiphysics family [16] according to prediction of structure creation refer to local phenomena modeling for very small separated zones without reference to whole casting and mould. There is generated grow of single equiaxed grain only or at most a group of some crystals (dendrites) usually in 2D without real conditions [17,18]. That can't have the application expected by practice even to simple shape ingots while considering the most complex shape castings it is even worth. Calcosoft CAFE tries to show the application direction. The sensitivity of model testing on the data base parameters to simulation was shown in this paper.

2. Ranges and variation of experimental and simulation conditions

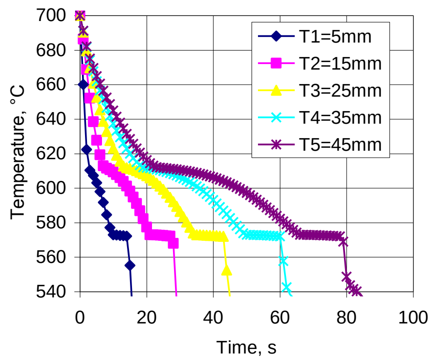
Locally heat extraction form casting depends on the set of applied mould materials. In this group – chill especially copper chill because of its thermal parameters belongs to the best heat receiver when we do not take into consideration the castings which are chilled by the die with cooling channels where inside flows cooling fluid [19]. In stationary sand moulds where there are applied chills the amount of heat accumulation depends on λ, c and ρ parameters and also on chill volume and contact surface between chill and casting. Exactly this surface sometimes limits the value of "aggregated" heat flux coming from the casting volume where it is necessary to obtain oriented and refinement structure with considerable mechanical properties.

The example of casting-mould (chill) system which enables to neglect the limited condition of surface contact and enables testing of chill influence without that restriction was shown in this paper. There was applied the cylindrical shape casting of 30 mm diameter i.e. relatively smaller than the one which was applied in our previous papers [13,20] and it was chilled from the face by large copper chill. In case of useful castings the realization of that kind configuration: small contact surface – large volume of chill is more difficult to realize by its real.

Experimental and simulation tests were taken on cylindrical shape casting of 30 mm diameter and 180 mm high made of AlSi7Mg alloy. The casting was made in double material mould from high-insulation (HI) material with large copper chill (Ch) located from the face of casting surface. The aim was to force the local structure orientation – columnar dendrites. Virtual structure parameters (α - phase only) were respected to columnar-to-equiaxed transition – CET and grain size.

The aim of the test was to give the answer if the CAFE – 3D model values parameters for the best fitted for larger casting i.e. 70 mm diameter [13,20] satisfactory fulfils comparison with real casting of smaller massiveness i.e. 30 mm diameter.
The tests were made in the same range of values parameters which were tested for 70 mm diameter casting [13,14].

a)



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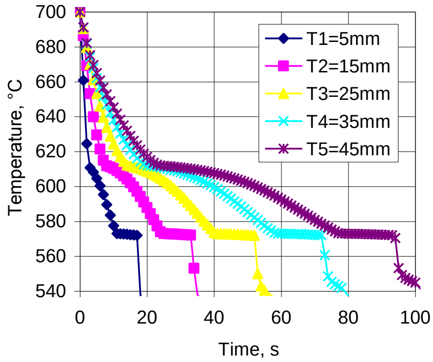


Fig. 1. Virtual cooling curves: a) casting ϕ30mm; compacted chill ϕ70x80mm, b) casting ϕ30mm; chill ϕ30x435mm; virtual thermoelements were located in the casting axis measured from the contact with chill

In order to indicate the presence of compacted chill significant with smaller casting contact there was realized additional simulation test. It was compared the influence of above configuration system – 30 mm diameter casting, chill ϕ70 x 80mm with the influence on the same 30 mm diameter casting but with contact surface of 30 mm diameter. Than the length of that kind of chill is 435 mm. The results which were shown in fig.1 and fig.2 and in table 1 indicate that energetic dimension of compacted chill in the place where there should be the best mechanical properties express good several percentages shorter time of solidification. Long chill with small transverse cross-section (massiveness obtained by length extension) in spite of very high λ, c and ρ of copper even λ higher than 300 W/(mK) doesn’t guarantee so fast heat extraction in the period when the primary structure are formed. The test confirmed more intensive influence of massive, compacted chill.

Table 1.
Virtual casting - ϕ30 x180mm solidification times, for two chills types: compacted ϕ70x80 mm (1) and long ϕ30x435mm (2)

Distance from chill surface, mm	Solidification time - τ, s		difference Δ, %
	casting ϕ30mm chill ϕ70x80mm	casting ϕ30mm chill ϕ30x435mm	*(τ₁-τ₂)/τ₂)*100%*
	τ sim (1)	*τ sim (2)*	
5	14	17	~18
15	27	33	~18
25	43	52	~17
35	60	72	~17
45	79	94	~16

a), b)

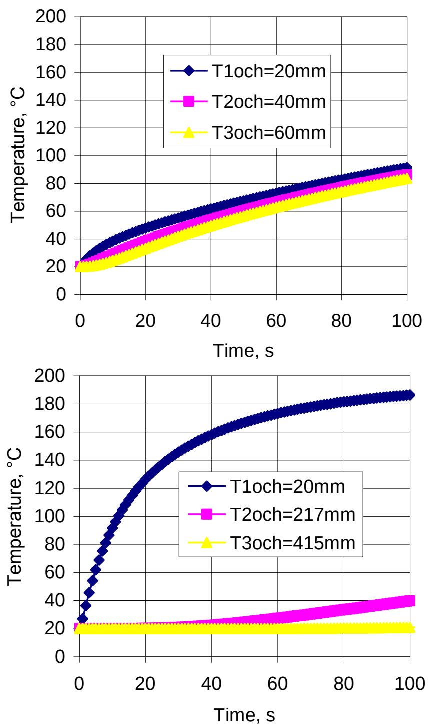


Fig. 2. Virtual heating curves of chill: a) casting ϕ30mm; compacted chill ϕ70x80mm, b) casting ϕ30mm; chill ϕ30x435mm; virtual thermoelements were located in the casting axis measured from the contact with casting

3. Tests results and analyze

Sensitivity test of model used in CAFE for cylindrical 30 mm diameter casting was preceded by chosen parameters which values were varied. The series of simulation tests with variation of particular values parameters were made (table 2). Procedure of CAFE – 3D model sensitivity estimation on the variation of particular parameters (look [13]) leading to model validation was based upon the only one parameter changing in each simulation test. There were no systematic interaction variations made.

Table 2.
Parameters used to simulation for casting realized in high insulation mould with chill (*bold*-variable parameter)

No	λ_{HI}	$\alpha_{casting-Ch}$	ΔT_{m-s}	n_s	ΔT_{m-Ch}	$n_{casting-Ch}$	ΔT_{m-v}	n_v	a_3
1	0,2	400	5	1e6	10	1e7	2	1e8	2,9e-6
2	0,2	400	5	1e6	10	1e7	**2,5**	1e8	2,9e-6
3	0,2	400	5	1e6	10	1e7	**3**	1e8	2,9e-6
4	0,2	400	5	1e6	10	1e7	**3,5**	1e8	2,9e-6
5	0,2	400	5	1e6	10	1e7	2	**2e6**	2,9e-6
6	0,2	400	5	1e6	10	1e7	2	**2e7**	2,9e-6
7	0,2	400	5	1e6	10	1e7	2	**2e9**	2,9e-6
8	0,2	400	5	1e6	10	1e7	2	1e8	**2,9e-5**
9	0,2	400	5	1e6	10	1e7	2	1e8	**2,9e-7**
10	0,2	400	5	1e6	10	1e7	2	1e8	**2,9e-8**
11	0,2	400	5	1e6	10	1e7	**4**	1e8	2,9e-6
12	0,2	400	5	1e6	10	1e7	2	1e8	**1e-6**
13	0,2	400	5	1e6	10	1e7	2	1e8	**6e-6**
14	0,2	400	5	1e6	10	1e7	**4,5**	1e8	2,9e-6
15	0,2	400	5	1e6	10	1e7	**6**	1e8	2,9e-6
16	0,2	400	5	1e6	10	1e7	**5,5**	1e8	2,9e-6
17	0,2	400	5	1e6	10	1e7	**5**	1e8	2,9e-6
18	**0,5**	400	5	1e6	10	1e7	2	1e8	2,9e-6
19	**0,8**	400	5	1e6	10	1e7	2	1e8	2,9e-6
20	**1,0**	400	5	1e6	10	1e7	2	1e8	2,9e-6
21	0,2	**800**	5	1e6	10	1e7	2	1e8	2,9e-6
22	0,2	**1000**	5	1e6	10	1e7	2	1e8	2,9e-6
23	0,2	**2000**	5	1e6	10	1e7	2	1e8	2,9e-6

Hard model parameters (all parameters are clearly described in [21]):
λ_{HI}- mean heat conduction of high-insulation mould, W/(m·K)
$\alpha_{casting-ch}$- mean heat transfer coefficient on cast-chill bound, W/(m^{2}K)

Soft model parameters (all parameters are clearly described in [21]):
ΔT_{m-s}- undercooling (high-insulation mould surface), K
ΔT_{m-Ch}- undercooling(chill surface), K
ΔT_{m-v}- undercooling (bulk of liquid), K
n_s- nucleation density (high-insulation mould surface), 1/m^2
$n_{casting-ch}$- nucleation density(chill surface), 1/m^2
n_v- nucleation density (bulk of liquid), 1/m^3
a_3- growth kinetics coefficient, m/(s·K^3)

Analysis and thermophysical (hard type model) coefficients selection and value parameters used in empirical relations (soft type model – nucleation and growth) required to simulation which lead to obtain good virtual to experimental structure conformity are easer in conscious selection of listed parameters when the influence of parameters on structure is known (model’s sensitivity).

The variation of liquid phase temperature field in crystallization process depends on casting-chill set and diversification of thermophysical mould materials parameters. Liquid and solid (solidified) phase temperature values are calculated in finite elements nodes according to classical thermal model of source transient field (macro-model). Temperature values are calculated in finite elements nodes and let to interpolate temperature in any point of space using so-called interpolation coefficients [22]. These points are assigned to cellular automaton nodes.

Mould thermophysical parameters which have high influence on temperature decreases of liquid phase are λ, c and ρ of mould material and heat transfer coefficient - α on contact surface (interface) between chill and casting.

Good conformity procedure of cooling curves and determined upon that basis solidification time for virtual casting in comparison to real one is in simplified way the method of inverse solution (trial&error metod). It is possible to estimate the λ, c and ρ values of mould material and heat transfer coefficient - α and lead to energetic validation of thermal model (assumption about constants of these averaged coefficients during the significant time for crystallization process).

Tests results of both value parameters groups influence on CET in CAFE model were shown in table 3. Tests results of significant value parameters influence of model: λ_{mould}, ΔT_v, a_3 – kinetic coefficient and n_v - grains density in the bulk of liquid and $\alpha_{casting\text{-}Ch}$ on CET were shown in fig. 3. These diagrams are useful for parameters selection during virtual to real structure fitting for cylindrical 30 mm diameter casting.

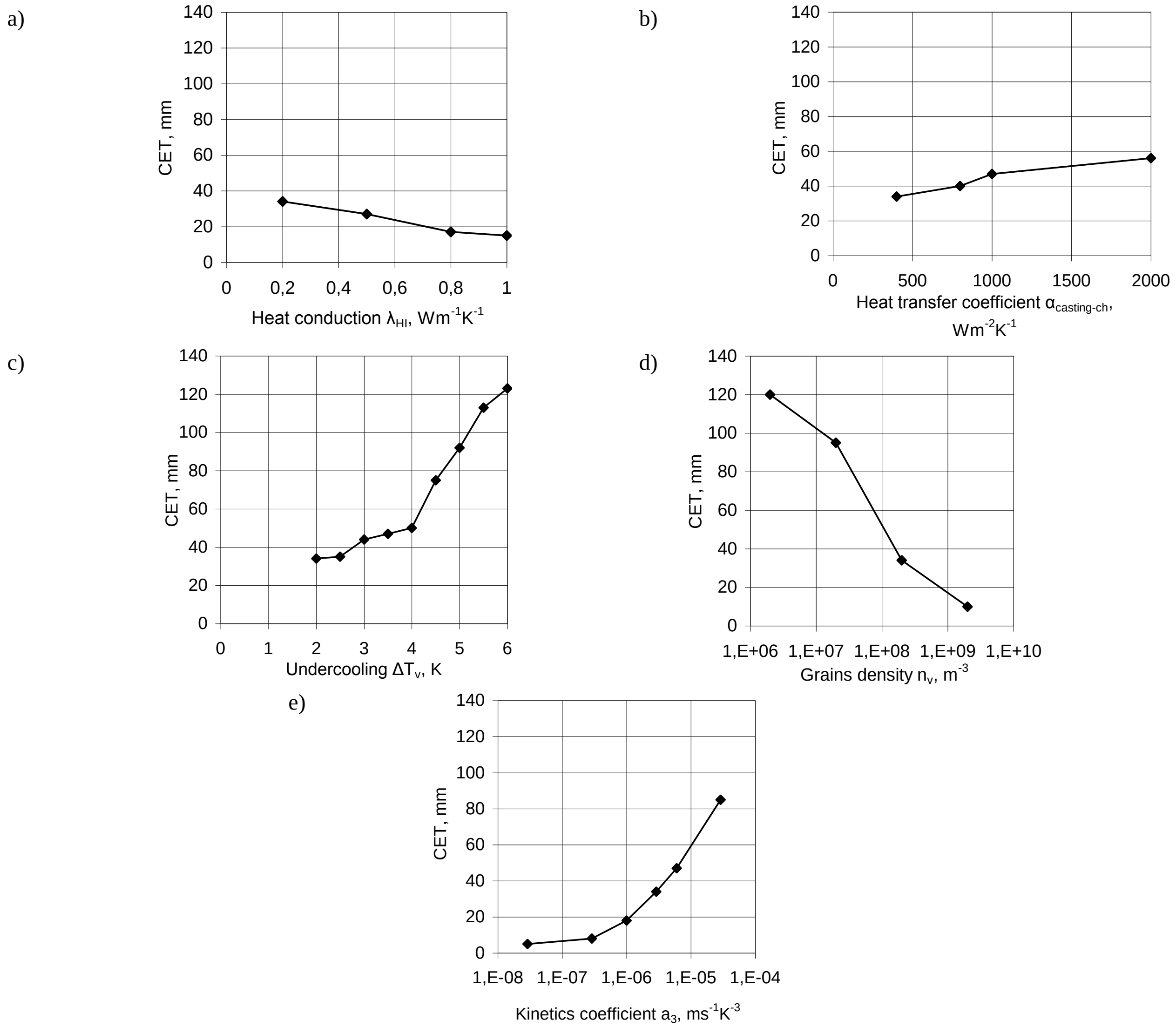
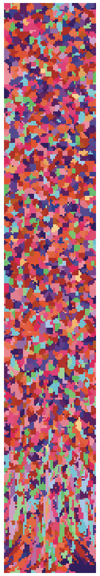
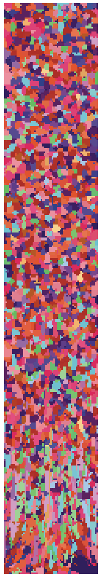
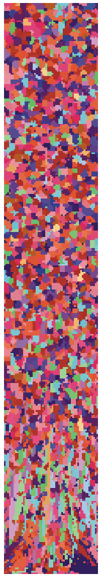
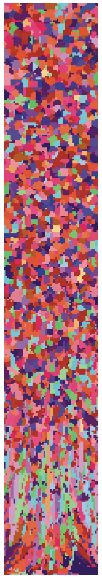
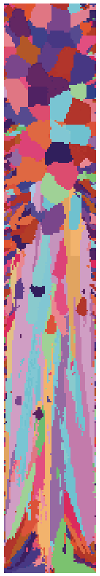
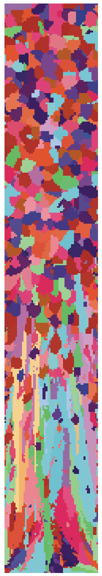
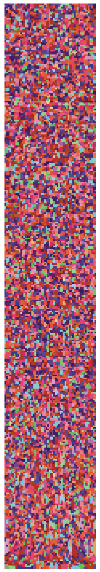
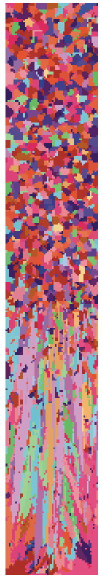
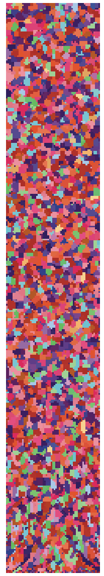
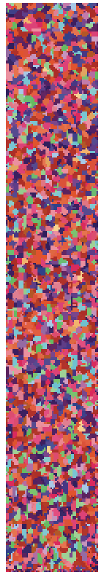
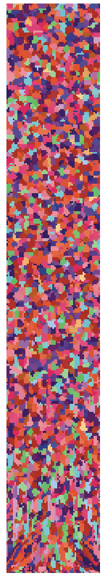


Fig. 3. Graphs of models' sensitivity on particular thermophysical and CAFE model parameters for 30 mm diameter casting (look table 2 and 3)

Table 3.
Virtual structures of cylindrical 30 mm diameter casting diameter (look table 2)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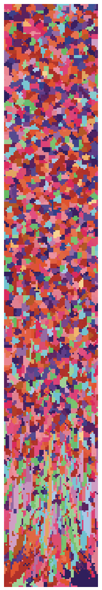		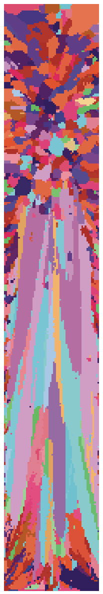	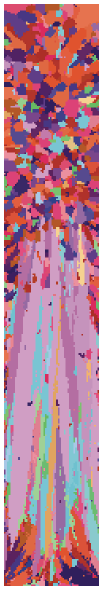	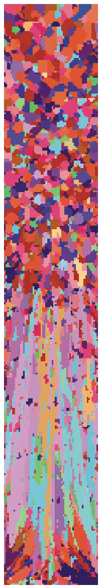	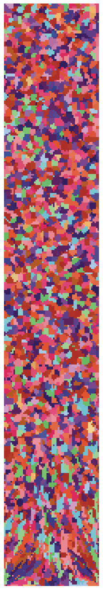	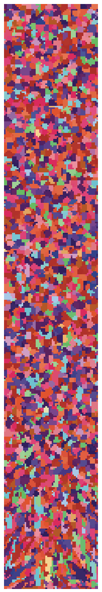	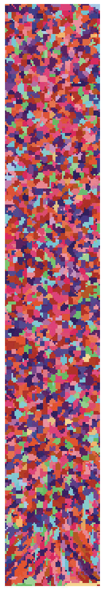	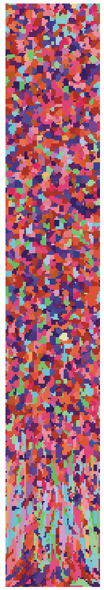	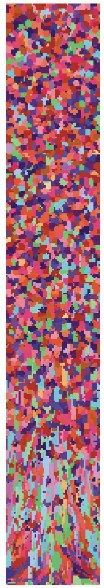		
13;CET=47	14;CET=72	15;CET=120	16;CET=113	17;CET=92	18;CET=27	19;CET=17	20;CET=15	21;CET=40	22;CET=47	23;CET=56	

Table 4.
Structure parameters (look fig. 3d)

Cross-section location	Virtual structure			Etched field on cross-section – real sample	
	Z=20mm transverse	Z=60mm transverse	Z=70mm transverse	Z=20mm transverse	Z=60mm transverse
CAFE structure parameters	columnar	equiaxed		columnar	equiaxed
Total grains number (Nb)	178	120	97	98	67
Grain density on the surface, 1/m^2	252 219	170 035	137 445	138 370	94 600
Mean grain surface, $F_{z\ śr.}$ mm^2	3,96	5,88	7,27	7,2	10,3
Ovalization indicator	0,45	0,49	0,52	-	-
Mean grain size $d_{z\ aver.}$, mm	3,35	3,9	4,23	3,0	3,6

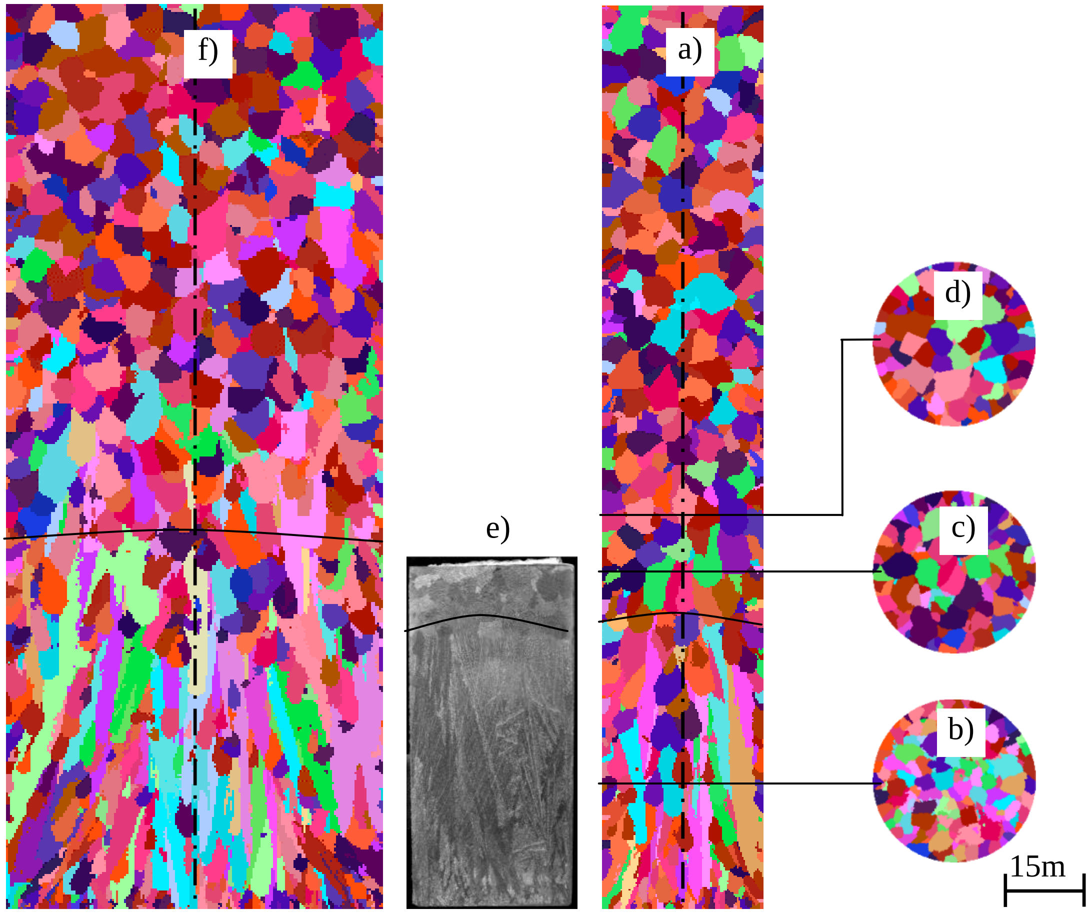

Fig. 4. Structure comparison: a - virtual and e) real cross-section. Etched by F5S20A20, additionally there are transverse cross-sections in the distance from cooled bottom of casting: b) Z=20 mm, c) Z=60 mm and d) Z=70 mm and f) virtual structure of ϕ70 mm casting (comparatively)

Structures set: virtual of cylindrical 30 mm diameter casting for the best value parameters obtained for the best fitted for 70 mm diameter casting [13] and experimental structure for cylindrical 30 mm diameter casting was shown in fig. 4.

Virtual structure parameters were shown in table 4. The average size of equiaxed crystals on the transverse cross-section (Z=60 mm) of virtual structure ($d_{z\ aver.}$= 3,9 mm) has good conformity with real structure ($d_{z\ aver.}$= 3,6 mm, difference lower that 10%).

The average grain surfaces on particular cross-section (fig. 5 a,b,c) were the base to estimate the average grain size using weighted average value of surface. The set of weighted average grains contribution values surface for transient cross-section with average surfaces in defined classes-intervals (look histograms – bar graphs) were shown in fig 5 d.

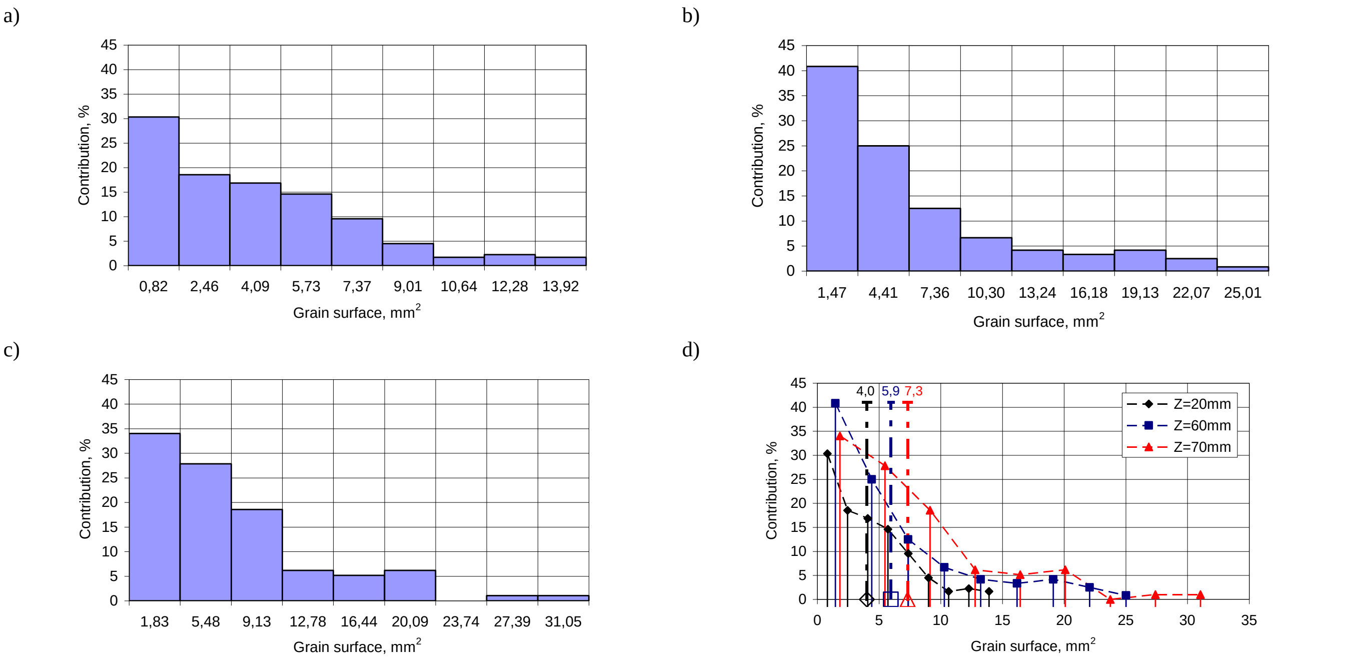

Fig. 5. Histograms of grains surface according to classes partition of virtual structure on transverse cross-section in the distance of Z: a) 20 mm, b) 60 mm, c) 70 mm, d) comparison of average grain surface counted by CAFE – 3D system and weighted average for 3 transverse cross-sections

Thermal "penetration" of cooling effect from compacted chill identified by using simulation reaches relatively deeper in smaller casting obtaining CET zone location of approximately 50 mm (fig. 5). In the real case CET zone location is approximately 54 mm, grain size 3,9 mm while average orientation of crystallites – 19° according to casting axis. Virtual structures visualization of cylindrical 70 mm and 30 mm diameter castings (fig. 4) indicates that on the virtual structure parameters of 30 mm diameter castings (70 mm diameter chill was used, for the same dimensions which was applied for 70 mm diameter casting) have influence the chill volume (compactness). Volume of 30 mm diameter casting – 137 cm^3 is more than 6 times lower than 70 mm diameter casting – 847 cm^3. Volume from the contact with chill to CET zone location so in that part where we found to obtain better mechanical properties there will be also proportionally lower. The effect should be better (lower values of DAS in real structure). Obtained virtual structure tests results for cylindrical 70 mm and 30 mm diameter castings for the same values parameters of CAFE – 3D model follow that estimated values parameters for the best virtual to real structure fitting of 70 mm diameter casting can be applied to structure parameters prediction of cylindrical castings in the range from 70 mm to 30 mm. Castings which diameter is lower than 70 mm the fitted structure validation can be realized by introducing the correction of n_v value (fig. 3d). While CET zone will be too low, it can be specified simultaneously according to pseudo-dendrite orientation increasing firstly a_3 (fig. 3e) and afterwards $\alpha_{chill\text{-}Ch}$ (rys. 3b). Above mentioned conclusion let us to expect about universality of assigned soft part model values parameters of CAFE model for casting – multimaterials mould set in the dimension range of tested castings.

4. Conclusions

Coupled modeling applying using hard and soft models it is necessary to understand the interactions on results and related with it proper values coefficients from pre-processing data base for both groups' models. Firstly it should be undertaken the energetic validation of system (hard model) leading to conformity of experimental and virtual solidification times supported by casting-mould system temperature validation [23]. The next validation stage is to lead to satisfactory conformity of structure parameters (soft model), variation only these parameters which have significant influence on simulation result. This is necessary during working with multiphysics family system to realize model's sensitivity testing according to method indicated in this paper and skillfully combined information: I type (gained during real time process) and II type (gained after crystallization process) [23]. There are some validation operations which indicate that final effect according to expected conformity with experiment can be realize by more than one parameter in addition from both models' types: hard and soft (e.g. $\alpha_{cast\text{-}mould}$ and a_3). In that case one should focus especially on methodological matters of experimental validation and to extend tests range. In [6,10] there were described the advices according to validation working which should enable individualization and optimization of system implementation which is enable to products quality prediction and interaction on manufacturing methods. Modeling extension about new coupled models has to be realized with keeping synergy rules of knowledge from many kinds of science and practice. At the end it should be pointed that limits of effective modeling have to be necessarily together with conscience of limitation and possibilities not only mathematical description (hard, soft) and resolvable conditions (mathematical, hardware). Extremely important is the range and method of reality simplification with analysis about their admissibility and effects which are carried. In that way only next fitting to new models from „multiphysics" group could be estimated according to real utility in foundry technology and development of that field.

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