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Examples of New Models Applied in Selected Simulation Systems with Respect to Database

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Abstract

The *tolerance of damage* rule progressively meets the approval in the design casting parts procedures. Therefore, there were appeared the new challenges and expectations for permanent development of process virtualization in the mechanical engineering industry. Virtualization is increasingly developed on the stage of product design and materials technologies optimization. Increasing expectations of design and process engineers regarding the practical effectiveness of applied simulation systems with new proposed up-grades modules is observed. The purpose is to obtain simulation tools allowing the most possible realistic prognosis of the casting structure, including indication, with the highest possible probability, places in the casting that are endangered with the possibility of shrinkage– and gas porosity formation. This 3D map of discontinuities and structure transformed in local mechanical characteristics are used to calculate the local stresses and safety factors. The needs of *tolerance of damage* and new approach to evaluate the quality of such prognosis must be defined. These problems of validation of new models/modules used to predict the shrinkage– and gas porosity including the chosen structure parameters in the example of AlSi7 alloy are discussed in the paper.

Keywords: Application of Information Technology to the Foundry Industry, Porosity and structure prediction, Databases, Thermo-physical parameters, Simulation codes, AlSi alloys

1. Introduction

In order to enhance the knowledge in scope of modelling and simulation in the foundry processes, one should be acquainted with the hard modelling based on physical-mathematical formula and also the soft modelling, burdened with simplifications resulting from both:` knowledge level on description of particular phenomena and level of theirs complexity. The trends observed in modelling of foundry processes and expectations of users compared with creators' upgraded propositions – new, additional modules based mostly on poorly tested theory have to be discussed. In such cases, each new module should be tested on sensitivity of additional parameters, which appear in extended database of these new modules. If needed and possible, these tests ought to be related to validation of the whole complex model containing such new modules.

The fundamental purpose of manufacturing processes virtualization, belonging to materials engineering group i.e. prediction of quality of final products like castings is achieved by modelling.

Coupling models of materials science with theories describing physical phenomena is obvious. It is essential to take into consideration the influence of given manufacturing process parameters and adopting values of these parameters in virtualization in applied models such as Fourier-Kirchhoff and other physical or/and empirical equations coupled with basic heat

transfer models [1]. It seems that a synergetic approach in these problems and developing works on thermo-physical databases in aspect of model description simplifications is necessary.

The paper considers the problem of usefulness of thermo-physical databases, characterizing the mould materials and heat transfer coefficients in casting-mould system during virtualization and used in order to carry out optimization of casting processes.

The sensitivity of simulation results depending on: variability of heat resistance (the effect of air gap formation on cast–mould or chill interface), the parameters describing mould material like heat conduction, an alloy density variation and modelling of latent heat release during alloy crystallization were analyzed.

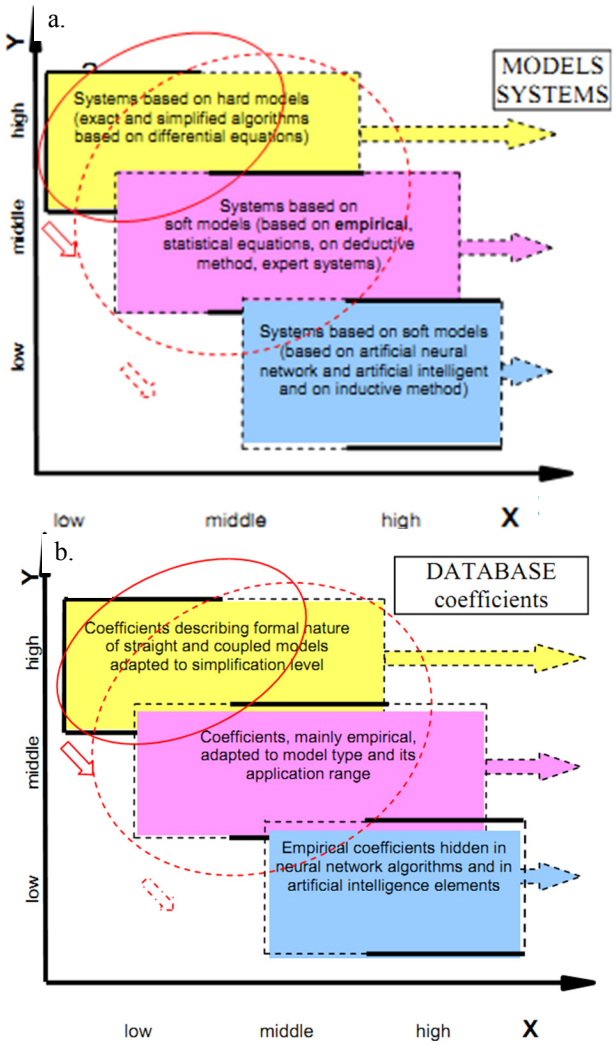
The validation of applied models was achieved on the basis of experimental cooling curves, discontinuities and .structure parameters.

The simulation tests were carried out for: AlSi alloy casting – copper chill system, obtaining coupled influence of temperature gradient and the crystallization interface movement rate in chilled zone. The validation was based on setting up the size of oriented structure zone called CET (columnar-to-equiaxed transition), which has textural character.

The multi-physics models [2] developed in order to increase the accuracy of prediction of porosity presence, not only of shrinkage origin but also the gas-shrinkage porosity, were put to the sensitivity analysis with variation of additional parameters applied in these complex models. The realized tests included also variation of the material parameters in database: density and castability (for shrinkage discontinuities) and variation of gas solubility (for gas porosity). The simulation tests were carried out using NovaFlow&Solid, Procast and Calcosoft simulation codes.

2. Reference to phenomena complexity in foundry processes and development of its modelling

Obtained gradient of physical (mainly mechanical) properties present in the casting depends on kind/size of metallic and non-metallic phases and structure discontinuities. Such "non-averaging" approach to the real casting in spite of obvious characteristic is the newest trend of optimization of casting materials features (the best adjustment of local casting strength to performance requirements) during the modern design stage, with the aid of *Integrated Engineering* methodology, taking into consideration the specificity of foundry engineering [3]. In order to consider all these complex phenomena, the coexistence of modelling methods and its validation is needed, as shown in the Fig. 1. Ellipses with arrows symbolize directions of expansion of synergy of model connections and innovative trends in virtualization development. Author's opinion on the connection of three models groups (simulation systems) captured in co-ordinates: level of phenomena knowledge – level of problem complexity. It is not technically possible to connect virtualization of processes in nano (atomic) scale with calculations in macro-modelling scale of the whole object – Fig.2 (e.g. cast-mould system) [4,5]. The macro-micro scales relations in known simulation systems are developed by application of soft modelling (e.g. nucleation and empirical models of crystal growth). Synergy of the three described groups of modelling is expected and should be constantly developed. This concerns not only physical data attributed to physical laws (describing specific phenomenon with differential equation) but also data operating on the linked coupling of empirical or/and neural models (or others criteria) [6].



Y – knowledge level about phenomena – possibilities of their description using physical- mathematical equations, X – level of problem complexity (phenomena, processes)

Fig. 1. Fields connection schemes in phenomena modelling in engineering virtualization process according to: a – models and systems, b – database – coefficients

3. Thermal, porosity and structure problems resolved by inverse solutions

The condition of effective use of simulation systems in practical applications is an awareness of simplifications used in model formulations. The scientists-creators of simulation codes constantly offer new and more complex descriptions of phenomena, but with symbolic experimental validation, their value has only a theoretical and postulate character. The

Fig. 3 contains a scheme of algorithm of simplified approach to inverse problem solution with usage of experiment.

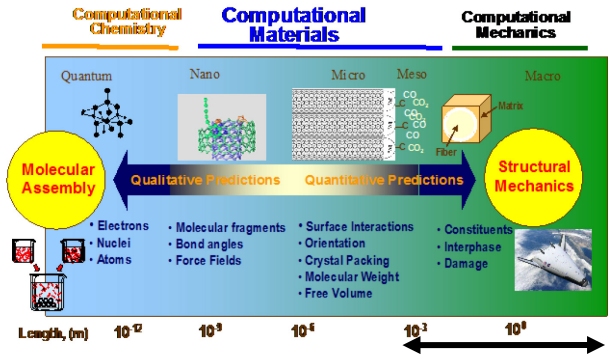


Fig. 2. Physical scales in materials and structural systems (from NASA Langley Research Center Nanotechnology Modeling and Simulation) [4] with indication of industrial virtualization utility borders (bottom arrow)

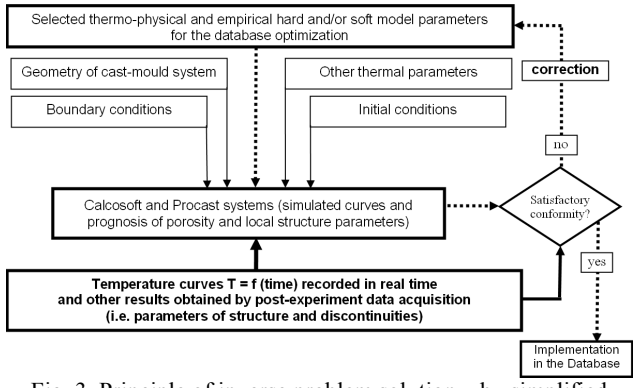


Fig. 3. Principle of inverse problem solution – by simplified try&error method (dotted line), applied to validate of modules described above and to complete of Database

4. Experimental tests and energetic validation

The experimental studies comprised of manufacturing the plates (thickness – 22 mm, height – 150 mm, width – 120 mm) and cylindrical (diameter 70 mm, height 220 mm) castings (Fig.4). Castings were manufactured in quartz sand moulds with copper chill and were made out of AlSi7Mg0,3 (AlSi7) alloy. Temperature measurements were performed using mantle thermocouple NiCr-Ni of 1 mm diameter with additional shield of chrome-nickel steel with 1,6 mm in diameter. The arrangement of the thermocouples is shown also in the Fig. 4 [7].

The chosen cooling curves obtained during experiments are presented in the Fig. 5. Measurements by extreme thermocouples: no 1 and 7 (15 and 135 mm distance from the chill) were a subject of comparative analysis. First derivatives $dT/d\tau$ indicate local solidification times of casting near the thermocouple no. 1 – t_s=49 s and the thermocouple 7 – t_s=264 s. The evaluation of thermo-physical data of mould material and heat transfer coefficient consisted in adaptation of simulation results to the experiment, in a way to achieve the conformity of calculations were realized using Calcosoft simulation code.

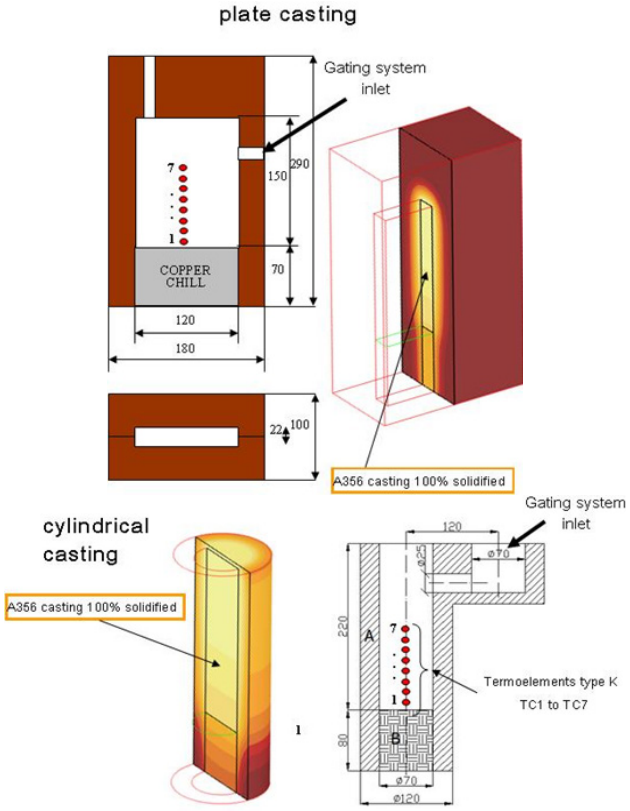


Fig. 4. Real and simulated experiments: sand moulds with Cu chill (with positions of 7 K-Th-couples – TC 1 to 7) [12,13]

As a result of inverse problem solution using iterative method, average value of the heat transfer coefficient of a cast – chill couple was determined – h = 1350 [W/m^{2}K]. Also, thermo-physical parameters of mould sand were determined – λ = 0,86 [W/m·K], cρ = 1,5e6 [J/m^{3}K]. For determined parameters, very good compatibility of solidification times between the experiment and the simulation was achieved (Fig.5). Determined parameters were put in the thermal database of all tested simulation systems (codes).

5. Modelling of phenomena of porosity formation and nucleation – crystal growth in foundry processes

After performing so called "energetic validation", metallographic examination was carried out and modules of NovaFlow&Solid – NFS CV, Procast and Calcosoft (Porosity and CAFE) systems were tested, in an attempt to answer the question about their sensitivity on variability of selected parameters. In Fig. 6 it was presented the selected results of the NFS CV simulation test of AlSi7 alloy casting applying the first of the

compared simulation codes. The obvious is the visible influence of the critical fraction on the final state of shrinkage discontinuities caused by density changes of AlSi7 alloy (T_{liq}=618°C, ρ_{liq}=2414 kg/m^3, T_{sol}=566°C, ρ_{sol}=2550 kg/m^3).

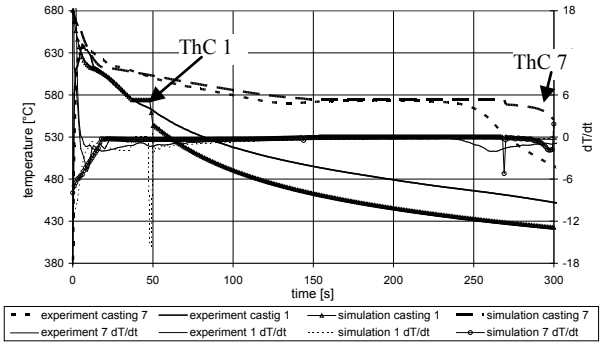


Fig. 5. Results of the real and simulated experiment – T=f(t) and dT/dt=f'(t) as the best conformity to the thermal macro-model (for chosen two thermocouples positions. Local solidification time TC 1: 49sec (exp&sim) and TC 7: 264 sec (exp) & 269 sec (sim).

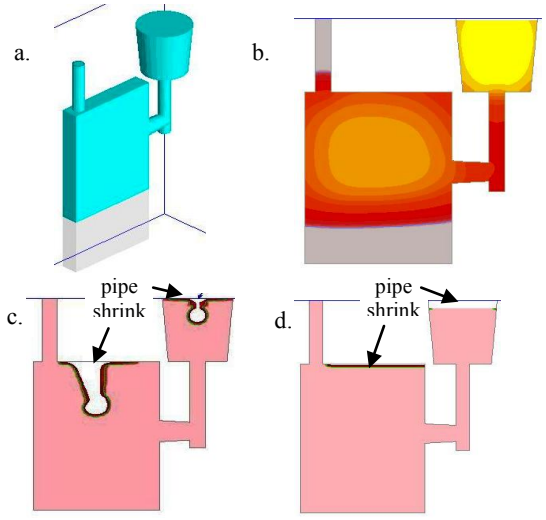


Fig. 6. Influence of critical value of solid fraction in database (NovaFlow&Solid – NFS CV): a – 3D geometry with bottom chill, b – location of hotspot, c – both fs_{crit}=0,2 (total shrink.1,5%), d – both fs_{crit}=0,7 (total shrink.4,9%)

The similar basic test for the database was performed for macro module Procast code, which allows the prediction of the location and intensity of the discontinuity of the shrinkage origin (Fig. 7).

Differsification of the AlSi7 alloy density in the range from the pouring temperature to T_{sol} in known manner decides about the demands for feeding metal .

The third tested code that uses new modules in comparison to the two previous modules (NFS CV and Procast) is a multi-module Calcosoft code (Csoft). The calculation results obtained from the Thermal module as the output is taken up by two tested modules: Porosity and CAFE.

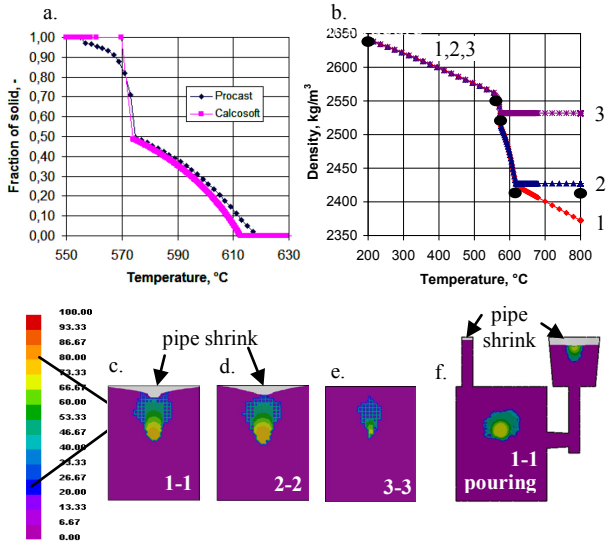


Fig. 7. The f_s=f(T) (a) and ρ=f(T) (b) applied to CS and Procast macro models tests– ρ variations for Procast: 1-1, 2-2 and 3-3 and for CS between the black points (• – •). Examples of shrinkage positions for 3 cases ρ=f(T) (c, d, e). Procast for critical piping solid fraction CPSF=0,3, critical macroporosity solid fraction CMSF= 0,7, f – shrinkage position (with pouring).

Fig. 8 shows the selected set of the results of one of the many tests which were obtained Calcosoft–Porosity module. For five selected moments of time the temperature, solid fraction and porosity part profiles are compared (in plate height). On this base the assumptions concerning porosity algorithm formation were arbitrarily defined by Calcosoft creators. This algorithm is not disclosed in details to users.

The principal parameters adopted for the simulation are shown in Table 1.

The Fig. 9 confirms the gradient nature of real gas-shrinkage porosity of the AlSi7 casing by Penetrating Testing (PT) – $PFPT=0{,}88e^{0{,}028x}$ [x, cm].

The presented validation of global porosity results calculated by Calcosoft and Procast Porosity modules are not satisfactory and require further work on these models improvement and experimental validation. Its practical usefulness has not been confirmed, especially regarding above cited *tolerance of damage* needs (procedures based on real 3D maps of casting structures/properties).

Fig. 10 presents effects of validation of CAFE module for the case of AlSi7 alloy casting with Cu chill (experiment described above). The differing parameters of CAFE module, shown in the Fig. 10, draw particular attention. The comparison of virtual-real structure oriented in the space and presented on the figures parameters of Calcosoft-CAFE module that the modelling of crystallization exists for the best fit of database special parameters (obtained by inverse solution) [8].

The Porosity and CAFE modules are described in the bibliography [9,10,11]. Its were also the subject of analyses during the research conducted by team of the authors [8,12,13].

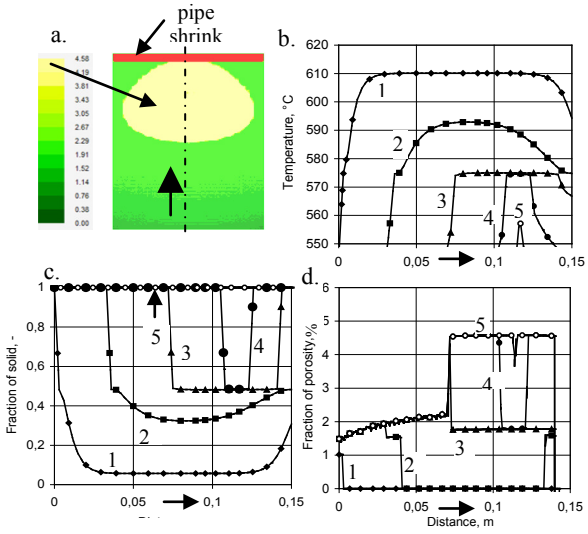


Fig. 8. The distribution of gas porosity in the function of distance from chill in casting (on the axe dash dot line): a – porosity distribution, b ¨temperature, c – fraction of solid and d – fraction of porosity in appropriate time moments: 1 – 10 sec, 2 – 61 sec, 3 – 130 sec, 4 – 178 sec and 5 – 183 sec.

Table 1.
Principal parameters of Database in Calcosoft – Porosity

Parameter	Name		Value (Calcosoft)
λ_{mould}	heat conduction of sand mould		0,86 W/mK
$C_{p\ mould}$	heat capacity of sand mould		1500 kJ/m^{3}K
$\lambda_{Ch\text{-}Cu}$	heat conduction of copper chill		390 W/mK
C_{pCh}	heat capacity of chill		3300 kJ/m^{3}K
λ_{AlSi7}	heat conduction of alloy	liquid phase	90 W/mK
		solid phase	130 W/mK
$C_{p\text{-}AlSi7}$	heat capacity of alloy (macro module)	liquid phase	3483 kJ/m^{3}K
		solid phase	2700 kJ/m^{3}K
L_{AlSi7}	latent heat of alloy		1,131·10^9 J/m^3
$\alpha_{cast\text{-}chill}$	heat transfer coefficient on cast-chill interface		1350 W/m^{2}K
T_0	initial alloy temperature in mould.		640 °C
Tz	pouring temperature (Procast)		720 °C
T_{Al}	melting temperature of pure Al		660,6 °C
T_{eut}	eutectic temperature		574 °C
c_0	initial solute concentration		7
k	partition coefficient		0,117
m	liquidus slope		-6,85
$\rho_{l,o}$	liquid density		2423 kg/m^3
ρ_s	solid density		2554 kg/m^3
ρ_e	eutectic density		2532 kg/m^3
-	mobility limit		0,2 – 0,7
CMSF	critical macroporosity solid fraction (Procast)		0,7
CPSF	critical piping solid fraction (Procast)		0,3
cc_{STP}	gas nominal concentration (max)		0,1 (0,5) ml/100g
k	gas partition coefficient		0,1

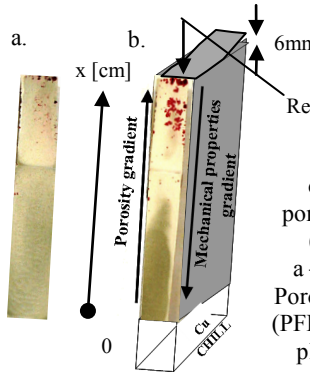


Fig. 9. Pipe shrinkage and distribution of gas-shrinkage porosity in the AiSi7 plate casting (by PT – penetrating testing, a – after 5 sec, b – after 15 sec). Porosity factor identified by PT test (PFPT, surf. %) in central section of plate casting varies with height PFPT=0,88e^{0,28x} [x, cm].

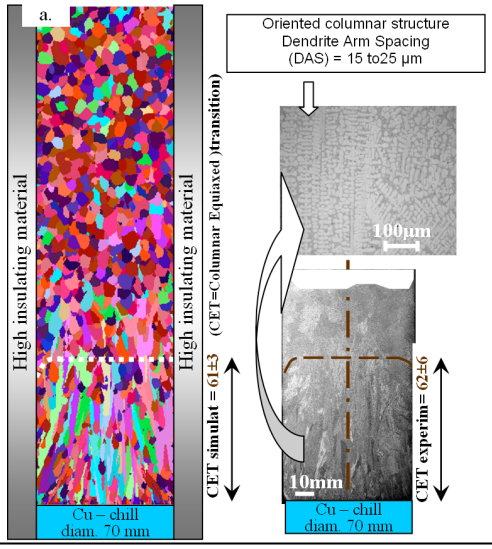
6. Conclusions

The *tolerance of damage* rule poses new challenges which consider the accuracy of prediction in relation to the actual structure state and its discontinuities and their combined impact on the local mechanical properties. The important trend which has to be developed is a reasonable introduction of new models. Each new module introduced as an expansion of existing models regarding a complex image of phenomena in cast-mould system requires a special approach to validation. The paper presents examples concerning modelling of the gas-shrinkage porosity and structure, than some of which are still widely used in industrial applications of virtualization. It appears that the prediction of shrinkage discontinuities require also the permanent validation and comparison with the results of adapted experiments. The expected possibilities of these modules were shown in confrontation with new challenges regarding databases for modelling of AlSi alloys casting processes. The methodology always used by the team of authors, consisting of connecting validation experimental study with numerical experiments, allowed to estimate a sensitivity of new modules to newly introduced and necessary parameters of the databases. Examples of validation described in the paper have also confirmed that the new modules (models) are sensitive only to some database parameters. It have also shown (e.g. porosity prognosis), that on this stage of validation only limited quantitative agreement with experiment can be achieved. The purposefulness of complicating the descriptions of elementary phenomena in these new modules and simultaneously about justification of applied model simplifications is very important.

These simplifications often result in subtle considerations originating from the physico-chemical analysis of the processes

being "unreadable" in simulation results or not confirmed after comparison with the results of validation studies.

The precipice existing between the worlds of macro-micro modelling (objects of size measured in meters to micrometers) and modelling in the nano (atomic) scale requires an intensive work in two areas. On the first side, there is a need to find a coherent physical description of phenomena from the macro scale to atomic scale: basic differential equations (hard modelling) and equations resulting from the empirical approach (soft modelling), but also, and maybe mostly on the other side – there is a need to develop microelectronics and new generation of computers (calculation speed and memory size).



Principal chosen parameters governing the heat transfer, nucleation and growth phenomena:

$H_{cast\text{-}insul}$ (heat transf.coef.)=10000 W/m^{2}K

$H_{cast\text{-}chilll}$ (heat transf.coef.)=2500 W/m^{2}K

1 - Empirical nucleation model – nucleation distribution (Gauss distrib.) [9,10]

$$\frac{dn}{d(\Delta T)} = \frac{n_{\max}}{\sigma_{\Delta T}\cdot\sqrt{2\pi}} \exp\left[-\frac{1}{2}\left(\frac{\Delta T - \Delta T_{N(s,v)}}{\sigma_{\Delta T}}\right)^2\right]$$

$\Delta T_{m\text{-}s}$(mean surf.undercooling)= 5K and $\Delta T_{m\text{-}s\text{-}Ch\text{-}HI}$=10

n_s (max nuclei surf.number) = 1e5 1/m^2 and $n_{s\text{-}Ch}$ = 8e5

$\Delta T_{m\text{-}v}$ (mean volume undercooling)=2K

n_v (max nuclei volume number)=8e6 1/m^3

$\sigma_{\Delta T}$=0.4 K

2 – Empirical dendrite growth model (Kurz-Giovanola-Trivedi) [9,10]

$$\upsilon = a_2\Delta T^2 + a_3\Delta T^3$$

a_2 (growth coef.) =2.9e-3 mm/(sK^{-2})

a_3 (growth coef.) =1e-9 mm/(sK^{-3})

Fig. 10. Simulated (CAFE 3D) and real CET zone for cylindrical Al7Si casting (ϕ70mm) solidified on the copper chill. The validation only limited quantitative agreement with experiment can be achieved

Acknowledgements

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