

## HEAT TRANSFER PROCESS COMPUTER SIMULATION AND MICROSTRUCTURE PREDICTION DURING CRYSTALLIZATION OF METAL ALLOYS\*

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**ABSTRACT.** Processes of crystallization during casting formation from aluminum alloys, steel and cast iron have been studied using 3-D computer simulation. Temperature fields of castings have been obtained and the microstructure distribution of these castings has been predicted. A comparison between numerical results and experimental measurement has been performed. It is proved, that the proposed approach is suitable for investigation and analysis of casting technologies.

**KEY WORDS:** Casting formation, computer simulation, casting structure prediction.

### 1. Introduction

Purposeful experiments of casting formation from different non-ferrous and ferrous alloys have been designed and carried out with respect to investigation of nano-modified metal alloys [1]. The casting processes has been studied by means of the mathematical modelling and computer simulation. The widely known comprehensive software package MAGMASOFT has been used for this purpose.

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The package is created by MAGMA Giessereitechnologie, Aachen, Germany [2]. The developing team of the company continuously improves and extends the package in collaboration with many scientific projects from different departments of the leading German institutes as Foundry Institute, Aachen, Max Planck Institute, etc. Mathematical models built in the software are continuously upgraded with the most essential developments (dissertations or scientific publications) in material science. The mathematical models are extended and improved to cover more phenomena and processes. The same concerns also the data base, which provides possibility to treat big variety of materials and casting methods, too. Generally acknowledged fact is that MAGMASOFT is beyond competition in connection with the built up data base. This way, it competes successfully with the most famous and powerful software from the branch as ABBACUS, PROCAST, ANYCASTING, NOVACAST, 3D-FLOW, LVM-FLOW, PATRAN, etc.

MAGMASOFT is a universal software product designed to simulate the essential physical processes of casting formation. It allows treating almost all casting methods used in the modern practice. This software has a 3D geometric modeller with a wide range of various geometric bodies and possibilities for large variety of operations over them like translations, rotations, scaling, extruding along an arbitrary contour, etc. These operations allow a quick and precise drawing of objects and systems with very complex geometry. MAGMASOFT simulates the filling of runner system and cavity of the mould with the melt under conditions maximally close to reality. The visualization of the mentioned above processes are facilitated by up-to-date instruments like X-Ray (transparency of the volumes), accessibility to every section of the casting-mould system, vector visualization, magnifier, modelling of turbulence and laminar flows, animation, colour coded visualization of all physical fields and trajectory visualization of melt particles (“Tracer”).

The software solves the three-dimensional temperature problem not only during the filling but also during the casting crystallization and simultaneously takes into account the phenomena in the two-phase zone. Some specific criteria functions are calculated for the prediction of the structure and mechanical properties of the casting, based on the so obtained temperature field and its derivatives. The most important and famous phenomenological criteria functions are calculated from:

$$(1) \quad K = C_0 \left[ (\nabla T)^\alpha \cdot \left( \frac{\partial T}{\partial t} \right)^\beta \cdot \tau^\gamma \right]^\delta,$$

giving the different particular values of the parameters  $\{C_0, \alpha, \beta, \gamma, \delta\}$ . Well

established correlation exists between such criteria functions and the mechanical properties of the formed casting [3, 4]. The most important and informative of them are:

- **Thermal gradient**  $G = \partial T / \partial x$  (obtained from equation (1) when  $C_0 = 1$ ,  $\alpha = 1$ ,  $\beta = 0$ ,  $\gamma = 0$ ,  $\delta = 1$ ) **and cooling rate**  $R = \partial T / \partial t$  (obtained from equation (1) when  $C_0 = 1$ ,  $\alpha = 1$ ,  $\beta = 1$ ,  $\gamma = 0$ ,  $\delta = 1$ ). The low values of these two quantities correlate strongly with the size of primary dendrites. The rougher dendrite structure worsens the mechanical properties of the casting and in the greatest degree – the plastic properties of the material.
- **Niyama criterion**  $N = GR^{-1/2}$  (obtained from equation (1) when  $C_0 = 1$ ,  $\alpha = 1$ ,  $\beta = -0.5$ ,  $\gamma = 0$ ,  $\delta = 1$ ). The low values of  $N$  indicate high probability of porosity.

The presented above tools of MAGMASOFT were applied to the investigation of experimentally obtained castings of non-ferrous and ferrous alloys. The results for the different cases are given below.

## 2. Computer simulation of non-ferrous alloy casting.

The geometry of the considered casting is shown in Fig. 1 in a 3D view. Standard aluminium alloy AlSi7Mg has been used for its forming. The used die is manufactured of steel X40CrMoV5\_1. and consists of four parts – a bottom permanent semi-mould, two side cores and an internal cylindrical core. All of them are shown in Fig. 2 in a 3D, too. The gravity casting is used. The cavity of the mould is filled up through one of the feeders.

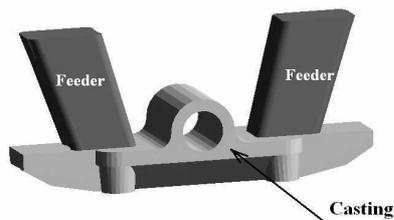


Fig. 1. Casting

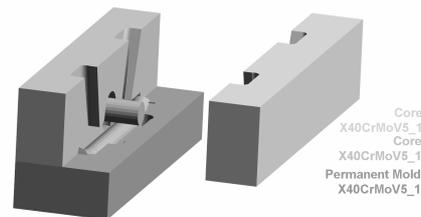


Fig. 2. Die

The processes of filling up and solidification of the casting are simulated with MAGMASOFT. Fig. 3 shows the temperature field at a moment of the mould filling up. The tool “Tracer” which visualizes the trajectories of some particles of the melt is shown in Fig. 4. This tool is very useful for tracing

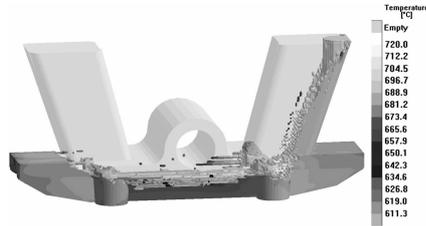


Fig. 3. Temperature field during the filling

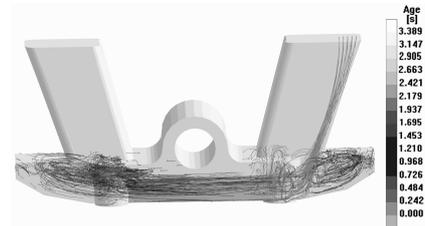


Fig. 4. "Tracer"



Fig. 5. Temperature field during the crystallization

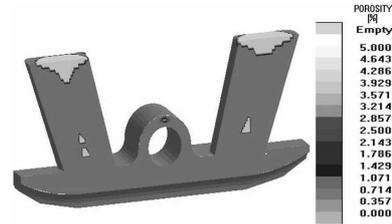


Fig. 6. "Porosity" criterion

of the nano-modifier particles during the form filling. The evolution of the temperature field during crystallization is also presented. A moment of it in the middle section of the casting can be seen in Fig. 5.

The solidus temperature has been taken for a lower boundary of the temperature scale. The "Porosity" criterion obtained by MAGMASOFT is shown in Fig. 6. It confirms, that the feeders are correctly designed and feed the casting successfully. Only a small problem zone is seen in the upper end of the ring-shaped part. The temperature field during the simulation is observed also in control points, which positions are given in Fig. 7. Point "T1" coincides with the thermocouple position. The curve denoted by T1-experiment in Fig. 8 shows the thermocouple indications. Other curves in Fig. 8 represent the temperatures in the control points obtained as a result of the simulation. Microstructure analysis of the produced castings has been made. The samples for this investigation are taken from the zones "1" and "2" pointed in Fig. 9.

The experimentally obtained average size of the secondary dendrites in these zones is shown in Fig. 10. On the other hand, Fig. 11 presents the predicted results for microstructure distribution, based on conducted simulations. Comparison with the experimental results shows, that the difference

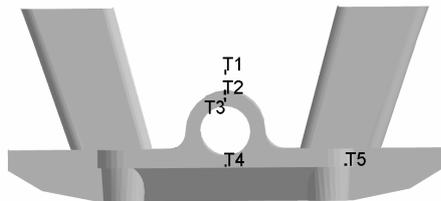


Fig. 7. Position of the control points

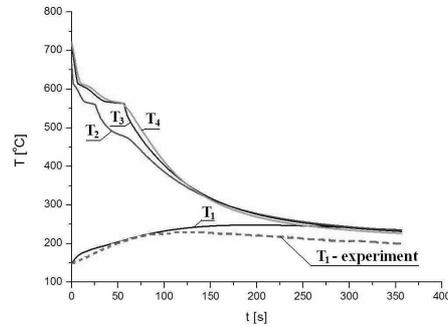


Fig. 8. Temperature curves – calculated and measured

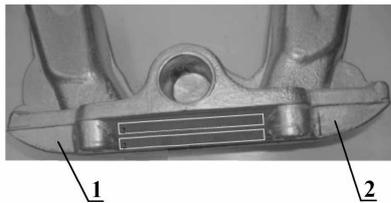


Fig. 9. Areas from which samples were taken for the analysis of microstructure

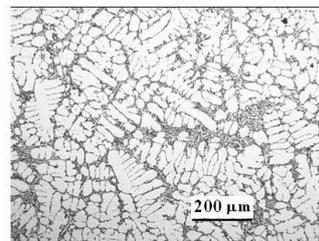


Fig. 10. Experimentally registered structure. DAS = 24 μm

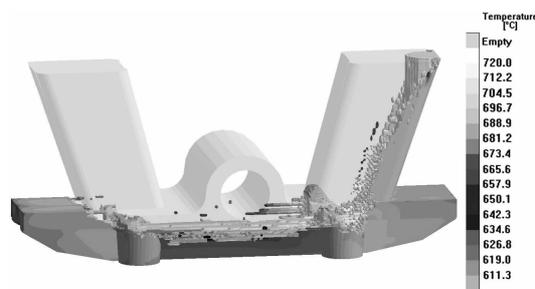


Fig. 11. Predicted structure

does not exceed 20% which is a completely sufficient accuracy for such kind of predictions.

### 3. Computer simulation of cast iron and steel castings

#### 3.1. Casting “Brake disk” of cast iron GG25

In contrast to the experimental casting mentioned above this casting is intended to the production of a component with practical usage – automobile brake disk. 3D geometry of the casting together with the runner system is shown in Fig. 12. The gravity casting in a sand mould is used, too. The mould filling up (Fig. 13) and solidification (Fig. 14) processes are simulated. The cast iron solidus temperature (1158 °C) has been taken for a lower boundary of the temperature scale in Fig. 14. Forecast for distribution of microstructure parameters into the casting have been obtained using computer simulations. They are shown in Figs 15 and 16. Figure 17 presents the experimental result obtained for the length of graphite lamellas registered in sample taken out from the place pointed out in Fig. 16. It is found a very good coincidence between forecast (Fig. 16) and experimental result (Fig. 17).

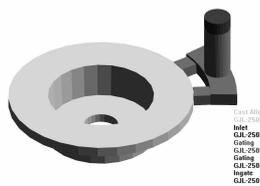


Fig. 12. Casting “Brake disk”

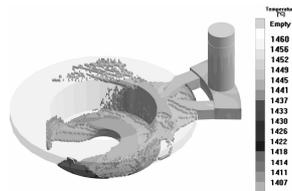


Fig. 13. Temperature field during the mould filling



Fig. 14. Temperature field during the solidification



Fig. 15. Average grain size

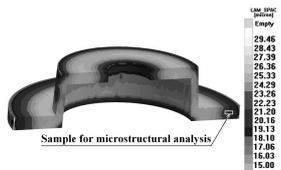


Fig. 16. Average length of the graphite lamellas

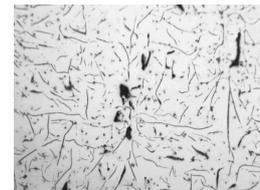


Fig. 17. Average length of graphite lamellas = 21 μm. Result of micro structural analysis

#### 3.2. Steel K20 casting

The geometry of this casting of steel K20 (C = 0.2%, Si = 0.45%; Mn = 0.7%) is given in Fig. 18.

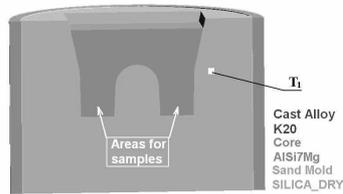


Fig. 18. Geometry of founder's equipment

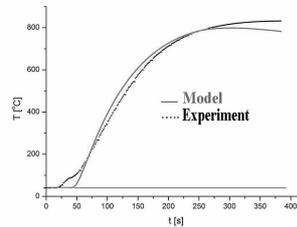


Fig. 19. Comparison between measured and calculated temperature

The computer simulation was carried out with the add-on module MAGMAsteel of MAGMASOFT. This module is specialized in steel casting. The temperature of control point  $T_1$  (Fig. 18) obtained by this simulation has a good coincidence with the measured one by the thermocouple mounted in the same point – Fig. 19. Figure 20 shows criterion “Porosity”. It evidences that the feeder is correctly dimensioned and the shrinkages caused by the mass deficit are out of the used for taking samples areas.

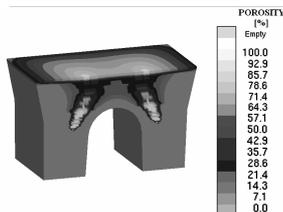


Fig. 20. Criterion “Porosity”

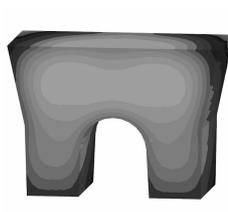


Fig. 21. Pearlite distribution

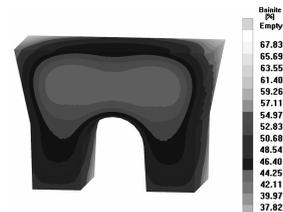


Fig. 22. Bainite distribution

The software allows to make predictions for the formed phase distributions, that in the case are mainly pearlite and bainite. The percent distributions of these phases are given in Figs 21 and 22, respectively.

#### 4. Conclusion

The given results presented above show that the chosen approach for simulation of the casting formation of various metal alloys has a sufficient degree of relevance to the real processes. Furthermore, they proved also that the proposed modelling tool is effective in predicting ongoing phenomena and properties of formed castings and can successfully be used and applied as appropriate tool in subsequent studies.

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