ANTAL KERPELY DOCTORAL SCHOOL OF
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Multiphysic multiscale numerical simulation of the solidification of binary and ternary alloys under forced convection

Thesis book

by
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1. Introduction

Aluminum and aluminum-based alloys are widely used in industry due to the corrosion passivity, lighter weight, yet – in several cases – comparable strength with steel. Often, the material is used "as-cast", that means that composition, macro- and microstructure of the material emerged during the casting define its behavior under different loads. Yet, convective flows generally arise in casting processes performed on-ground because of gravity. They modify local solidification conditions, and, consequently, solute distribution and affect properties of material. To understand and to be able to control such phenomena, detailed experimental and numerical work has been needed.

Two Bridgman-type furnaces were constructed in the University of Miskolc, Hungary, by MTA-ME Materials Science Research Group in the framework of the ESA funded MICAST project for experimental study of the effect of convective flow in solidification of alloys. These facilities were equipped with electromagnetic systems capable to generate rotating and travelling magnetic fields of various intensities.

Multiphase models developed at SIMaP/EPM, Grenoble, France, were applied for numerical study of the solidification of binary and ternary aluminum alloys under electromagnetically generated convective flow. Solidification of a binary Al-Si alloy under RMF stirring was done with Euler-Euler ensemble averaging and lever rule mesoscale models coupled with the macroscale transport both in 2D and 3D geometries. Further, effect of various modes of TMF stirring during solidification of a ternary alloys was studied in 3D geometry with lever rule based macroscopic model. Results of numerical simulations well explain the segregation observed in the experimental samples.

The aim of the current thesis is to numerically simulate the solidification cases realized with the experimental facilities equipped with travelling or rotating magnetic field stirrers in Miskolc and validate the results with the experimental data of MTA-ME Materials Science Research Group.

2. Experimental results of Miskolc

The presented experimental results are used later in the thesis as reference and / or validation values. The measurements were performed and published by other associates of the research group. The results were transferred for free usage in the simulations.

2.1. RMF experiments

In 2007 Kovács et al. performed experiments on Al-7Si-0.6Mg alloy using various magnetic field intensities. For the thesis project 20 mT magnetic induction was chosen based on the experience coming from the pure flow simulations. Such induction results in a flow of transient zone regarding turbulence. The used solidification model is designed for laminar flow, but a more intense test was in interest. The sample was provided using 99,99% base materials and cut into 8 mm mean diameter and 100 mm length.

During the experiment, the temperature data of the 13 thermocouples were collected and saved. It will be used as a boundary condition in the simulations. The plot of the dataset can be seen below.

The concentration distribution was also measured by Kovács et al. The result can be seen on the diagram below, but it is not showing clear enough the expected effects based on the etched samples. Therefore, a repetition of the measurement was essential with the aim of higher accuracy, since the currently available measurement devices have significantly better resolution. Moreover, the simulation results have helped in the design of the new measurement method.

The concentration distribution of 20 mT RMF sample was done on 3 longitudinal sections: 0-19 mm, 25-45 mm and 50-70 mm using the Edax EDS microprobe of a Zeiss electron microscope. A measuring window of 0.8 x 1 mm was chosen. Using this window, the whole sections could be mapped – 10 images across the diameter times 20 across the height. The first window was adjusted "by hand" to the proper position and then the automatic mechanism of the table was used to map the whole sample. The complete window area was measured so the values should be used as averages of an area of 0.8 x 1 mm.

Due to the morphology of silicon, the X-ray spectra had to be compensated. For that the cross section of an unmixed sample was used. The concentration has been measured and the resulting peaks were indicated as 7% Si and 93% Al.

The samples are a bit conical, so the last images do not completely cover the window, but it doesn't affect the accuracy of the measurement.

2.2. TMF experiments
2.2.1. Thermal effect in TMF

During the first experiments (performed by Arnold Rónaföldi) using the TMF facility, a yet unknown thermal effect occurred. The phenomenon is appearing the strongest way in case of the "XY" field configuration, when one side of the melt is pushed upward, the other one is pushed downwards. All the experiments start with an isothermal holding state when only the technical thermal gradient is set up and no lowering of the sample or mixing is used. The simple aim of this is to melt everything completely and have a complete thermal equilibrium in the system.

Regardless if there is sample lowering or not, at the moment of switching the stirring on, the thermal gradient crashes and a new one appears.

The experiment was performed for 5. 10, 20 & 40 mT, but 40 mT is the most spectacular one.

2.2.2. TMF experiments on solidification

A series of experiments were performed using the new TMF inductor – by A. Roósz, A. Rónaföldi and A. Jenő. The key force field is the "bi-directional" which is pushing the melt's two side upward and downward, since this is provides the strongest and most directed Lorenz force field. Al7Si1Fe alloy was used for the experiments on various inductions: 0, 20, 40, 80. For the current research, the 20 mT was chosen, since its flow field was validated via the thermal effect which was presented in chapter 2.2 and it is laminar (the current solidification solvers are not tested on turbulent flow). The main technical parameters were:

- Sample lowering velocity V_{sample} 0,05 m/s
- Thermal gradient G 5 K/mm
- Frequency f 50 Hz
- Magnetic induction B_0 20 mT
- TMF form XY bidirectional

The concentration distribution was measured with image analysis method. A mosaic image was provided of a cross section of the sample and two different areas were chosen. The left are shows higher Si content based on eutectic fraction. Such fraction was measured on the image and the Si content was calculated based on the phase diagram. The result of the two blue areas are

3. RMF simulations

The main technical parameters important for simulation are the magnetic induction, frequency and the temperature field dataset. Using the data of temperature field has great advantages for the models. The thermal gradient, sample movement velocity, thermal fluctuations are stored in the dataset. If the field is applied on all the walls of the crucible, no special treatment is needed for the boundary conditions and no effort is needed for the simulation of several experimental parameters. Four models were provided for the same experiment with comparison reasons. These were:

- 2D axisymmertical case using Envelope method for solidification modeling
- 3D model using Envelope method for solidification modeling
- 2D axisymmertical model using Lever rule for solidification modeling
- 3D model using Lever rule for solidification modeling

The application of solidification modeling into Fluent is done at SIMaP/EPM Laboratory (Grenoble, France) since approximately 2007 by Ciobanas, Noeppel, Fautrelle, Budenkova and Du Terrail. For Envelope method, an averaging structure must be applied since the model itself is written for the growth of a single grain, but one mesh cell can contain arbitrary number of growing dendrites and every cell can have different temperature, concentration, etc.

The solution is called ensemble averaging and was designed by Ciobanas et al. The system of equations is rebuilt in an averaged form and modified to compute on phase ratios instead of radii of solid, interdendritic liquid and extradendritic liquid phases. The model itself is written in a user defined scalar in Fluent. When the scalar, which contains the solidification model is computed, the iterations of it are performed. Using such approach every time step has sub time-steps with sub-iterations resulting in a "dual-layer" model. Ansys Fluent was chosen to be the main environment for the calculations due to its strength in complex heat and mass transfer solutions. The flow model was used as it is included in the program with momentum sources for the above described Lorenz force field.

Two models were prepared for two purposes. First is to see results on the experiments of Miskolc using Envelope method, and second, to see if the 3D modeling has any advantage compared to 2D axisymmetrical. 2D models were already published by Budenkova et al. in collaboration with MTA-ME Materials Research Group. The model was using Lever rule in a 2D axisymmetrical case.

Both cases were transient using Eulerian-Eulerian model for the multiphase problem. The two phases were solid and liquid. The solid is modeled as a liquid phase with ultrahigh viscosity – 1 Pa·s. It helps the convergence of the models.

One can observe that one more liquid phase is needed for the usage of Envelope approach. The Eulerian liquid phase is the sum of inter- and extradendritic liquid.

The two phases share the same temperature field and have the same flow parameters. The concentration is also treated in a shared and averaged form. For the diffusion problem between the phases, Ciobanas developed his own approach, which was used in the current work.

The growth model including the diffusion and concentration conservation law is calculated in a user defined scalar. The calculation is done iteratively with a self-written code provided by the French Laboratory.

The original energy model of Fluent is not used, but a self-written system is provided to be able to better treat heat fluxes, latent heat, eutectic reaction and the effect of the flow. The temperature data of the 13 thermocouples is interpolated (in time and space) on the walls as fixed values for every time step.

The 2D case was modeled in a rectangle of 4x100 mm meshed with 40000 quad cells (100x100 µm cells). For 3D, a cylinder of Ø8x100 mm was used meshed with 605000 hexahedron cells.

Regarding the flow, the four models show very similar results – as was expected from the setup. The form of the flow is identical, and the magnitude is very close to each other. The maximal velocity can differ which is the result of the difference in the 2D and 3D approach. These results prove that no difference should be considered due to the flow.

2D Envelope
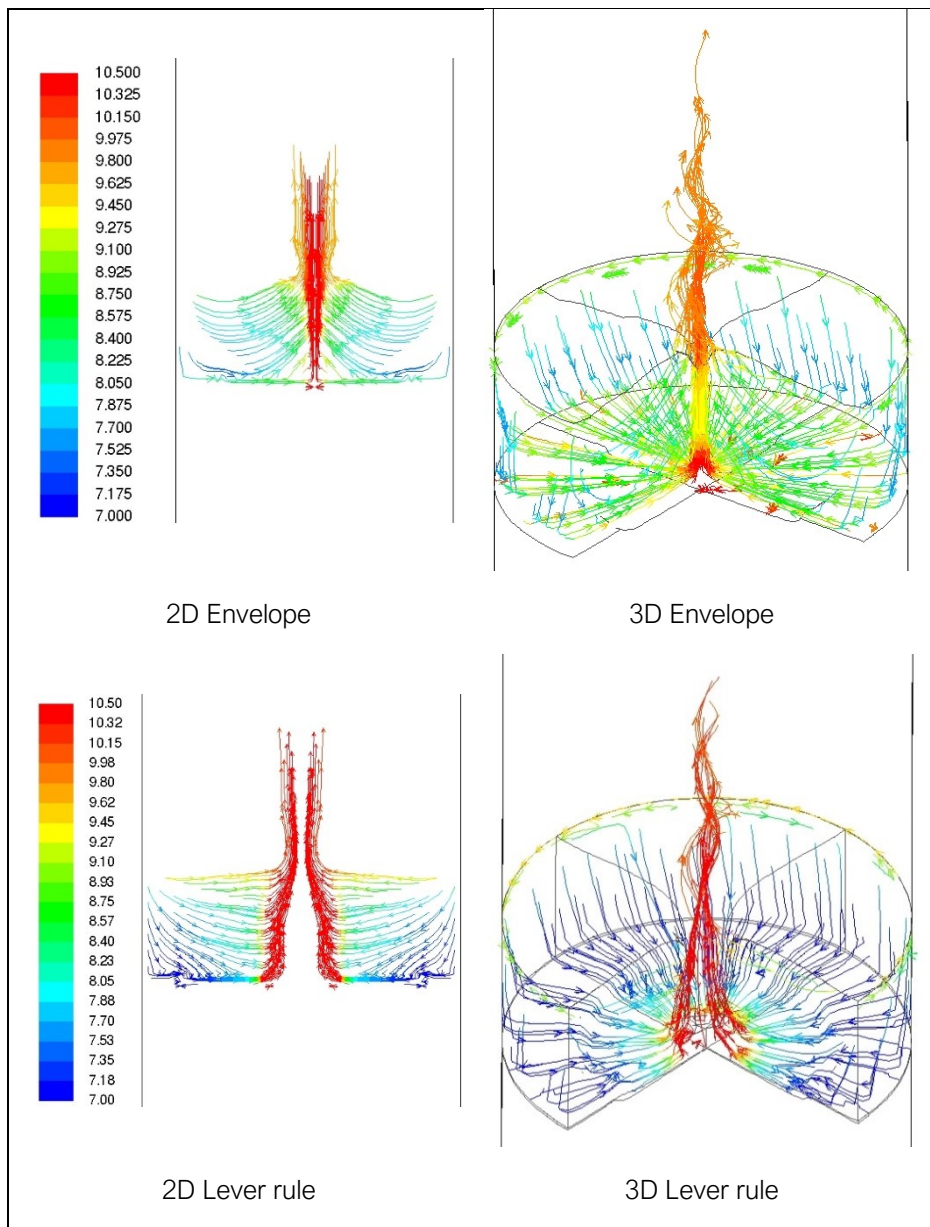
3D Envelope

2D Lever rule

3D Lever rule

Figure 1. Pathlines of velocity magnitude starting from the mushy zone – colored by average Si concentration [wt.%]

In point of view of 2D vs. 3D cases, no significant difference appears. Since the flow field is quasi-axisymmetric, there is no real advantage of building up a more robust case which requires higher calculation resources and longer time.
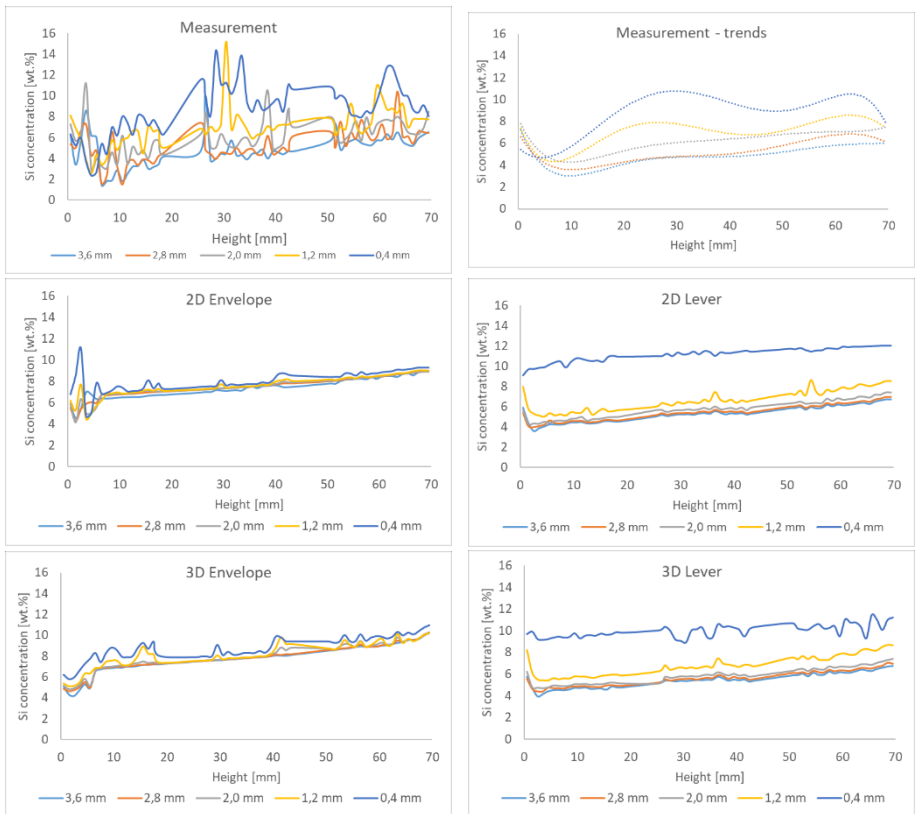

Figure 2. Si concentration plots as a function of height – at different axial distances

4. TMF simulations

4.1. Lorenz force field simulation series

A simulation series had to be provided to achieve the Lorenz force field, before starting the solidification simulations. The force field was validated via a thermal effect – gradient shift after turning the electromagnetic field. The first model was a pure electromagnetic simulation to achieve the Lorenz force field. The simulation resulted in qualitatively correlating results, but further validation had to be done. The second model was about the thermal system of the global experimental setup. The measured temperature distribution was applied on the furnace wall and the sample temperature was tracked. After reaching the correct stationary temperature, the heat fluxes appearing on the sample wall were saved. Such fluxes were included into a thermal-flow model together with the Lorenz force field of the electromagnetic model. As a result, the final thermal gradient shift effect was achieved and the Lorenz force field was ready for use in the solidification modeling.
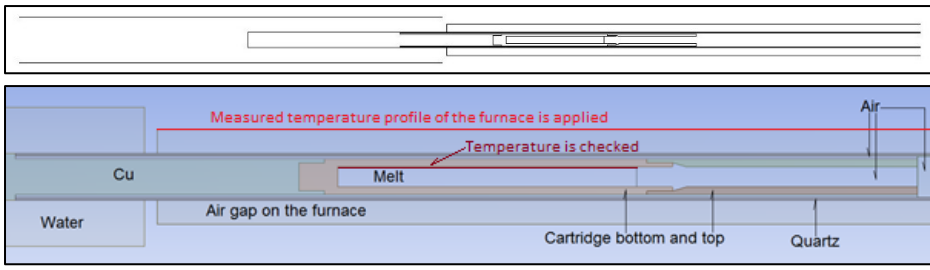

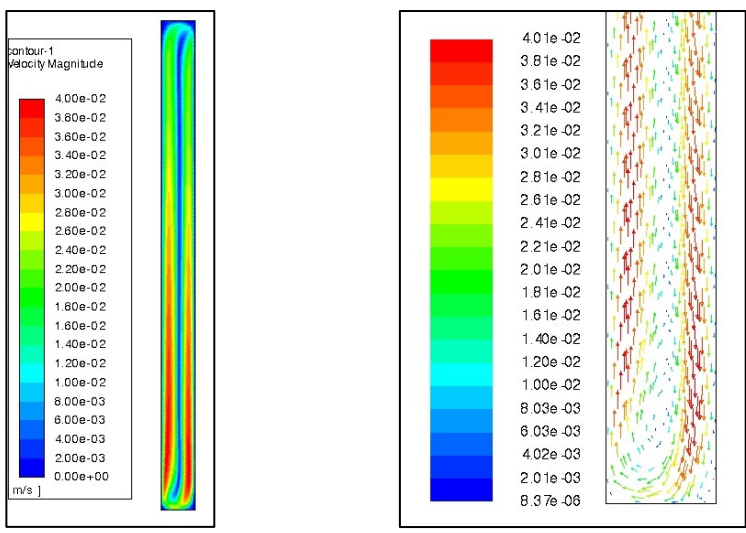Figure 3. The geometry of the global thermal model

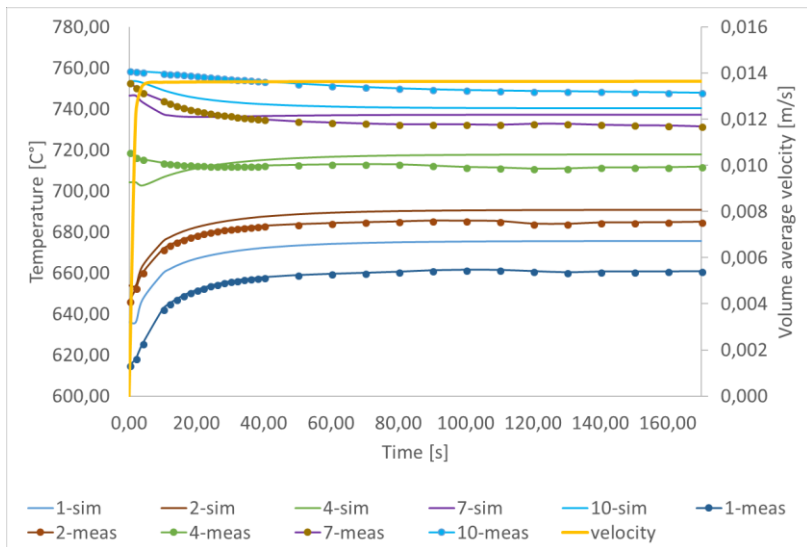Figure 4. Contours and vectors of the flow colored by velocity magnitude

Figure 5. Gradient shift after the adjustment of the flow field and settlement of the flow (maximal velocity)

4.2. Solidification simulation with bidirectional travelling magnetic field

On figure 6, the Si concentration distribution (on 30 mm) is compared with the texture image of the measurement (actually from 90 mm height). The simulation could not be finished to reach the 90 mm height, therefore qualitative comparison was possible only – and the results are promising, since the qualitative correlation is clear. The effect of primary and secondary flow is visible.
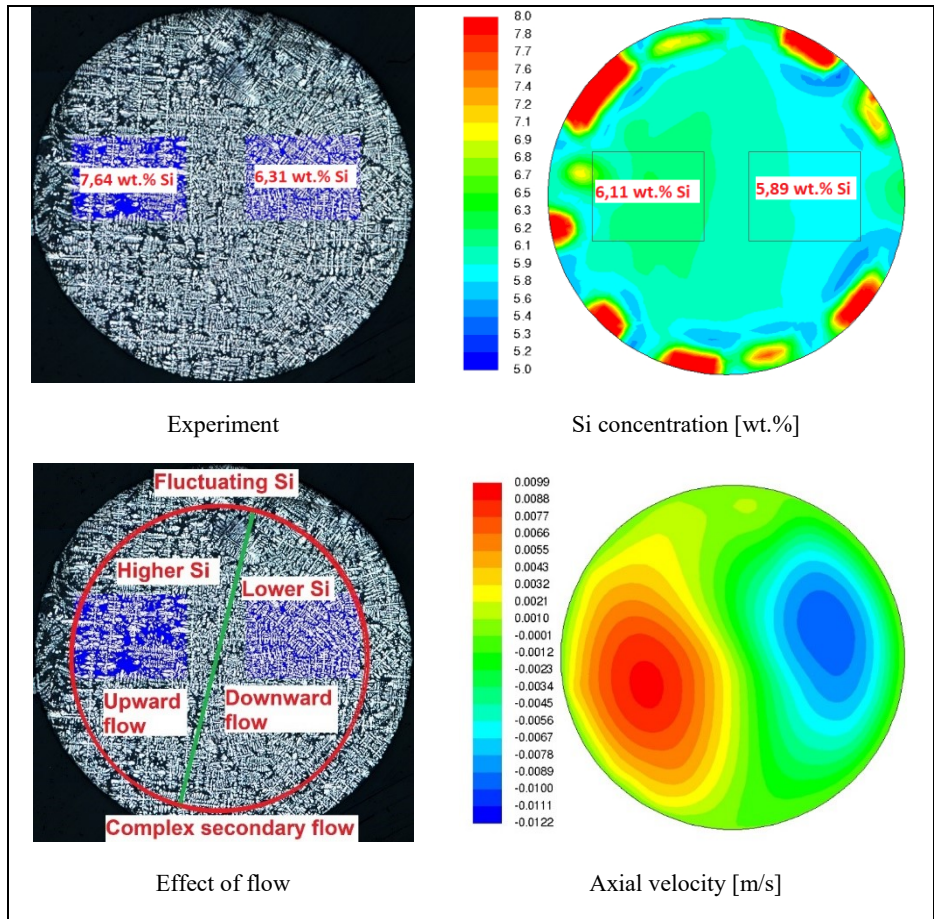

Figure 6. Effect of the flow field on the Si concentration distribution and comparison with the measurement

5. Scientific results of the project

Thesis 1:

Coupled multiphysics CFD RANS k-ε and magnetic force 3D simulation of solidification under rotating magnetic field in a cylindrical medium has no advantage and additional information compared to 2D-axisymmetrical cases. The flow field is quas-iaxisymmetric, and the solute distribution has no major difference, but the computational time longer or requirements are much higher in 3D case. The computation time of 3D is approximately 5-10x on a same hardware. For such simulations, 2D axisymmetric computations are recommended.

Thesis 2:

Coupled multiphysics CFD and magnetic force simulation of solidification under rotating magnetic field in a cylindrical medium, the Envelope method of solidification compared to Lever rule has weaknesses for higher volume of solidifying metal. The solute distribution shows qualitative correspondence with the measurements, but quantitatively there are either large differences. On the other hand, this problem did not occur with Lever rule. The Lever rule is an explicit analytical computation which fulfill the necessary conservation rules itself. In contrary, the Envelope model is an iterative computation, which incorporate an accuracy to, or on other hand a deviation from the conservation phenomena. The comparison of measured and calculated concentration fields suggests the application of Lever rule.

Thesis 3:

The directly unmeasurable flow patterns appearing inside the TMF Solidification facility designed and constructed by MTA-ME Materials Science Research Group at Miskolc, Hungary can be simulated and validated with the same multiphysics simulation as presented at RMF case. A thermal gradient shift effect was measured by 13 thermocouples of the facility. The geometry and the model were exceeded with the whole facility, and the measured temperature distribution was calculated too. Based on the comparison of the measured and calculated temperatures the validation of the flow is possible due to the strong connection between the different phenomena. The validation can be continued via the solute distribution resulting in the solidification modeling. Qualitatively the computed concentration field fits to the microstructure of the experimentally crystallized sample. This proves that this method of validation of such a complex multiphysics simulation gives the scientifically desired result. The same computation facility gives the same quality of computation either a TMF or RMF simulations.

6. Publications

O Budenkova, C Nagy, Y Du Terrail Couvat, S Steinbach, A Roosz, Y Fautrelle : Comparison of the 2D and 3D Simulation ofy Solidification of Binary and Ternary Al- based Alloys under RMF. Proceedings of the 6th Decennial International Conference on Solidification Processing. Old Windsor, UK, 2017.07 London: Brunel University, 2017. pp. 284-287. (ISBN:978-1-908549-29-7)

Csaba Nagy, Olga Budenkova, Yves Du Terrail, Yves Fautrelle, András Roósz: Effect of Electromagnetic Stirring on the Solidification of Al-7wt%Si Alloy: Experiment and Simulation. EPM 2015 Proceeding. Cannes, France, 2015.10.12-2015.10.16. Cannes: Centre National de la Recherche Scientifique (CNRS), 2015. pp. 77-80. (ISBN:9782955386101)

Nagy C, Fautrelle Y, Budenkova O, Rónaföldi A, Roósz A: Numerical simulation of the RMF stirring of molten Ga-In alloy using RANS k-ε and LES turbulence models. MATERIALS SCIENCE FORUM 790-791: pp. 402-407. (2014)

Csaba Nagy, László Gyulai, Arnold Rónaföldi, András Roósz: Investigation of the hydrodynamic properties of magnetically stirred molten gallium-indium alloy by numerical simulation. MATERIALS SCIENCE AND ENGINEERING: A PUBLICATION OF THE UNIVERSITY OF MISKOLC 38:(1) pp. 41-50. (2013)

C Nagy, A Rónaföldi, A Roósz: Comparison of measured and numerical simulated angular velocity of magnetically stirred liquid Ga-In alloy. MATERIALS SCIENCE FORUM 752: pp. 157-166. (2013)

Nagy Csaba, Yves Fautrelle, Olga Budenkova: Numerical simulation of the RMF stirring of molten Ga-In alloy using RANS k-ε and LES turbulence models. Sixth International Conference on Solidification and Gravity. Miskolc-Lillafüred, Hungary, 2013.09.02-2013.09.05. Z-Press Kiadó, p. 136.

Nagy Csaba, Roósz András, Rónaföldi Arnold, Gyulai László: Mágneses fémolvadék-keverés numerikus szimulációja. microCAD 2012, N section: Fluid and Heat Engineering (Áramlás- és hőtechnika) ISBN:978-963-661-773-8)

7. Conclusions

The current industrial needs for high quality aluminum require detailed knowledge of the phenomena arising during the processing of the materials. Without gathering information about the solidification conditions of a complex casting part, or a pre-product, like a billet for rolling, unexpected and unwanted failures can appear. To have a clearer picture on solidification processes, the work on the simulation of aluminum solidification under forced magnetic induction was presented in the thesis work.

The experimental work of other scientific groups was mentioned including the possibilities for numerical investigations. The numerical models were presented in more details, since those were used as basis of this project including magnetohydrodynamic background.

The results on RMF and TMF experiments performed on the special facilities of Miskolc were discussed. Those results were the validation keys of the project. In case of RMF field, enormous amount of experimental data is available including the thermal dataset of each experiment. The macrostructural images, concentration maps and temperature datasets were used as validation points or boundary conditions. The temperature field monitoring during the experiments provided a great advantage to simulate a thermal system accurately with the smallest effort possible so far. The qualitative accuracy of the models is surprisingly great. Moreover, in case of Lever rule approach, the quantitative conformity is really promising.

More complex simulation system had to be built up for the TMF facility due to its innovative design. Since the Lorenz force field cannot be directly described with any parametric equation, electromagnetic simulations were performed using Comsol Multiphysics. The results of the simulations were directly validated using the measurement results of the magnetic induction vector components close to the inductor heads, but it is not directly connected to the induced Lorenz force field.

To be able to validate the magnetohydrodynamic effects, the thermal gradient shift phenomen was used. The global thermal system of the complete facility was simulated for the heat fluxes on the crucible wall, which was interpolated in a thermal-flow model. The latter simulation was performed to quasi-validate the results of the MHD system. After several adjustments and introduction of the reduction factor for the Lorenz force field, the gradient shift effect could be simulated with great accuracy.

Solidification simulations were also performed for the TMF field using a ternary approach. Two models were presented: using bidirectional and upward Lorenz force field. Qualitative comparison was possible only for the bidirectional case, since the preparation of the samples were not possible in time for the upward case. The solute distribution conforms well with the resulting macrostructure.