

Modelling of Material Properties - A Viable Solution to the Lack of Material Data in Casting Simulation

Z. Guo^{1*}, N. Saunders¹, E. Hepp² and J.-Ph. Schillé¹

¹ Sente Software Ltd., Surrey Technology Centre, Guildford GU2 7YG, U.K.

² MAGMA Gießereitechnologie GmbH, Kackerstraße 11, D-52072 Aachen, Germany

ABSTRACT

Casting simulation requires accurate and reliable material property data, including the fraction solid transformed, specific heat capacity, thermal conductivity and density, all of which as a function of temperature. Such data are usually gathered from experimental sources, which has significant disadvantages in that not all of the required data is available, measurement of high temperature properties is expensive, and furthermore the properties can be sensitive to microstructure as well as to alloy composition. A modelling route that can calculate reliably all the relevant material properties would be of great benefit.

This paper briefly describes the development of a computer software JMatPro that can provide reliable and cost-effective material data required in casting simulation for multi-component commercial alloys. The property data calculated by JMatPro has been used as direct inputs to casting simulation software MAGMASOFT[®]. The focus of this paper is to examine how changes in composition within the specification range of an alloy may affect its properties during solidification, and how casting simulation results are consequently influenced.

INTRODUCTION

Casting process simulation is now widely accepted as an important tool in product design and process development to improve yield and casting quality. Such simulation requires high quality information concerning physical and thermo-physical properties during solidification. Some properties have been measured for specific alloys, but the number of alloys for which information is available is limited. Furthermore, the information may be incomplete in the sense that not all properties have been measured and, sometimes, disparate information from a variety of sources is used to build up the database for one specific alloy. The latter situation can lead to inconsistent results, as the composition of the alloys used for database creation may not be the same and consequently critical temperatures, such as for the solidus and invariant reactions, may differ between the alloys. To overcome the lack of data and provide reliable and cost-effective data for process simulation, as well as achieve a better understanding of how changes in composition within a specification range of an alloy may affect solidification properties, it is highly desirable to develop computer models for calculation of the thermo-physical and physical properties of multi-component alloys during solidification.

Within the framework of the development of the computer software JMatPro, extensive work has been carried out on the development of sound, physically based models for material properties [1,2]. Not only are these properties wide ranging, including density, volume, coefficient of thermal expansion, thermal conductivity, Young's/shear/bulk moduli, Poisson's ratio, viscosity, specific heat, latent heat and enthalpy, but also they are given from room temperature to the liquid state [3,4,5,6,7,8,9]. JMatPro also provides detailed information on the properties of each individual phase, such as the liquid phase in the mushy zone [3], which is usually beyond the capability of measurement. It is the aim of this paper to examine how changes in the composition of an alloy within its specification range affect properties during solidification, and how properties of the liquid vary in the mushy zone. To make JMatPro's calculated material data more easily used by modellers, the data can now be organised

* Corresponding author: Tel: +44-(0)-1483-685475; fax: +44-(0)-1483-685472.
E-mail address: z.guo@sentesoftware.co.uk

in such a format that can be directly read by casting simulation packages. Such linking has been successfully developed between JMatPro and the casting simulation package MAGMASOFT® [10,11].

JMATPRO CALCULATION

This section examines how changes in the composition of an alloy within its specification range affect properties during solidification using aluminium alloy A319 as an example. The composition of various A319 alloys is given in Table 1. Variations in elements Si, Cu and Zn were considered. The freezing range calculated from JMatPro for the three alloys were also given in Table 1.

Table 1: Composition and freezing range of three A319 alloys within the specification (wt.%)

A319	Si	Cu	Mg	Mn	Zn	Fe	Al	Freezing range (°C)	Remarks
Low spec	5	3	0.3	0.5	0.1	0.6	bal.	508-617	Lower limit of specification
Average	6	4	0.3	0.5	0.3	0.6	bal.	505-607	Average composition
High spec	7	5	0.3	0.5	0.5	0.6	bal.	500-596	Upper limit specification

Figure 1 shows fraction solid vs. temperature plots calculated for the three A319 alloys. As might be expected, with increasing Cu and Si the freezing range decreases, Table 1. Higher levels of Si also increases the amount of silicon eutectic and reduces the range of primary aluminium phase. It should be noted that for A319 alloy of high specification, the first solid phase formed during solidification is the intermetallic phase α -AlFeMnSi. However, the liquidus is taken as the solvus temperature of the Al phase as the amount of α -AlFeMnSi is small, forming as isolated intermetallics that have little effect on the casting behaviour of interest here. The change in density during solidification for the three alloys is shown in Figure 2, which reflects the fact that total density change is strongly affected by the fraction solid behaviour.

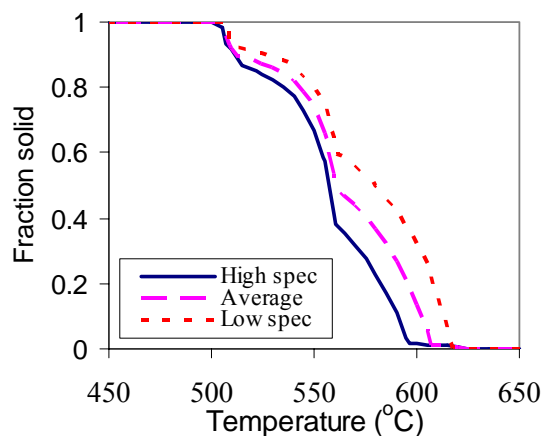


Figure 1. Calculated fraction solid vs. temperature for the three A319 alloys

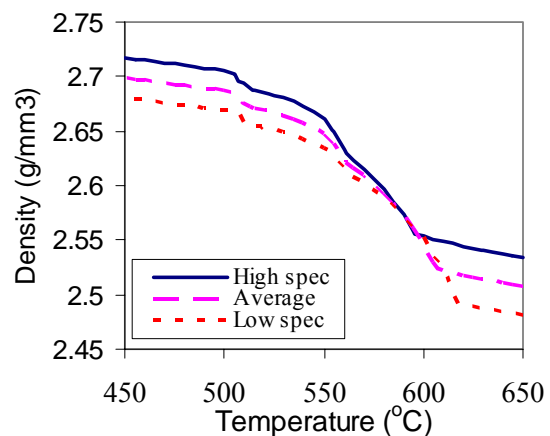


Figure 2. Calculated density vs. temperature for the three A319 alloys

Alloys with much smaller composition variations can produce quite substantial variations in the properties of the liquid within the freezing range. Aluminium alloy A356 is taken as an example here, with one composition being Al-0.01Cu-0.2Fe-0.3Mg-0.02Mn-7Si-0.025Zn (wt%), and the other of slightly higher levels of Cu (0.25%), Mn (0.3%) and Zn (0.35%). It is fairly easy to understand that the material properties will be different when the fraction solid curves of alloys differ a lot. However, in this case, the difference in fraction solid vs. temperature behaviour is less pronounced over most of the solidification range. However towards the end of solidification there are significant differences. For the low impurity alloy, solidification is complete at 556°C. At the corresponding temperature the high impurity alloy has 4% of liquid remaining and solidification is not complete until 540°C

There is also a quite substantial difference in the behaviour of the liquid during the final part of the solidification. Figure 4 shows the density changes of the A356 alloy with lower Cu, Mn and Zn. For this composition, there is a slight density inversion as Mg segregates into the liquid below the silicon eutectic. However, when Cu, Mn and Zn levels increase the behaviour of the liquid in the mushy zone changes dramatically (Figure 5). The initial dendritic Al solidification is very similar; however the behaviour during the eutectic part of solidification is quite different, with the liquid phase now being much denser. The viscosity is also strongly affected and both effects will affect liquid flow in the dendrite arms and hence defect formation.

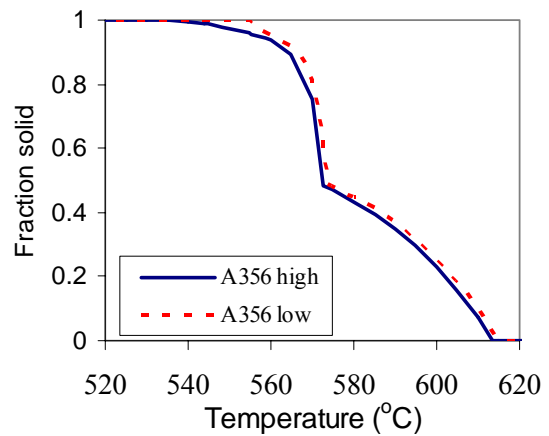


Figure 3. Calculated fraction solid curves for A356 alloys with variation in Cu, Mn and Zn.

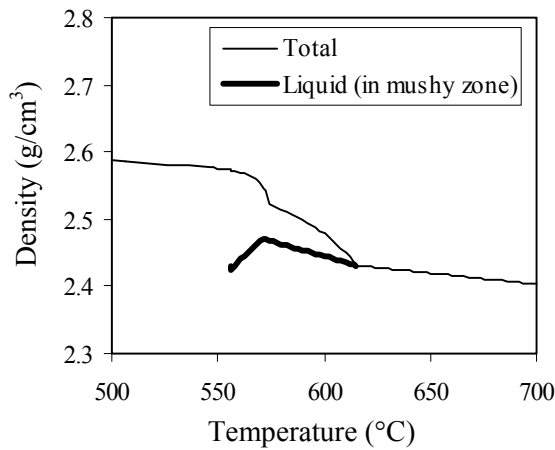


Figure 4. Calculated density of A356 alloy (with lower Cu, Mn and Zn) during solidification.

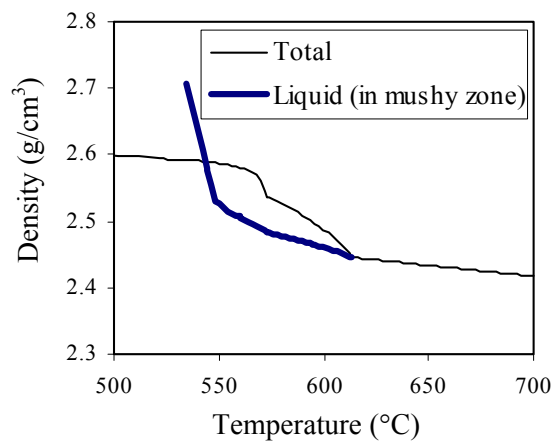


Figure 5. Calculated density of A356 alloy (with higher Cu, Mn and Zn) during solidification.

MAGMASOFT SIMULATION

This section examines how changes in material properties due to composition variation can affect the casting simulation results, via a study on casting simulation of a cylinder head typically made of A319 alloy using MAGMASOFT, based on the three compositions given in Table 1. Hotspot simulation of alloy A356 was also carried out to see the effect of smaller variations in Cu, Mn and Zn on a step for trucks. These two components are of different casting process. The cylinder head is from gravity casting, whereas the truck step is from high pressure die casting.

1, Alloy A319

Temperature at the end of filling

Figure 6 shows the calculated temperature field at the end of filling for the three A319 alloys. Of interest are the regions where possible coldflows can take place. The temperature scale in the pictures is set as a range from solidus to liquidus. The blue regions (circled) are places that are already below solidus just after finishing the filling, which could lead to coldflows. As can be seen although overall behaviour is largely the same, the alloy of the low specification has more “cold” regions than the other two alloys.

Local solidification time

Local solidification time is one of the most used criterion functions that can show potential regions for defects. Such regions are usually the isolated maximums in the casting. Figure 7 shows the calculated local solidification time for various A319 alloys. The pictures are from a different viewpoint from that of Figure 6. There are no isolated maximums, however, it can be seen that solidification behaviour has been significantly altered through changing the composition, which has a subsequent significant impact on the feeding behaviour in critical regions of the cast.

Feeding / Porosity

Figure 8 shows the calculated feeding percentage for various A319 alloys, which allows the user to determine the quality of feeding of the casting, which in turn will allow the user to see potential areas where porosity may occur (areas which have less than 100% dense). It can be seen that for the alloy A319 at high specification the feeding result shows no problems in the displayed region, while the average and low composition indicate potential problems with porosity. This can be explained due to the fact that for the best case, the local solidification time in the critical area is increased, leading to better liquid flow and hence a lower susceptibility to defects from poor feeding.

2, Alloy A356

Figure 9 shows the hotspot simulation results based on the properties of A356 with different amounts of Cu, Mn and Zn. Although the overall effect of changes in composition on fraction solid are small in comparison to the 319 alloys, significantly different behaviour is predicted to occur in the formation of isolated hotspots, leading to potentially significant differences in defect formation between the two cases. At this stage it is only possible to speculate on the exact reason for the behaviour. However it is clear that, during final stages of solidification, both the physical properties of the liquid and fraction solid behaviour are significantly different between the alloys.

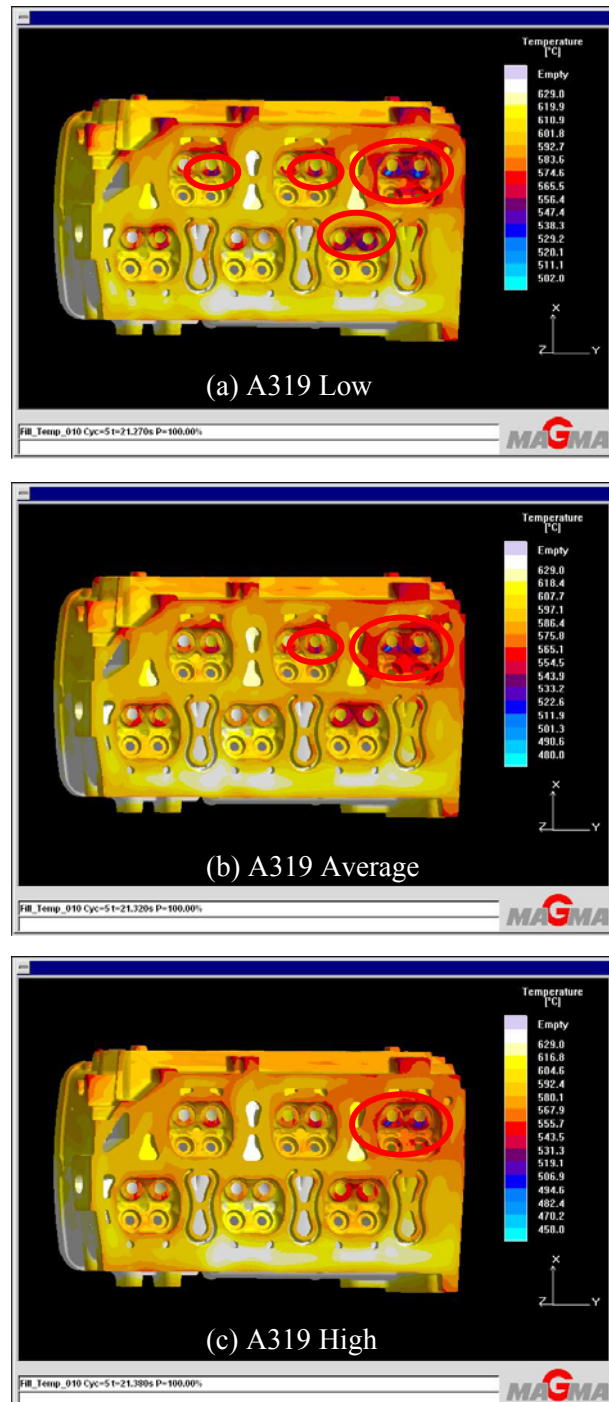


Figure 6. Calculated temperature at the end of filling for various A319 alloys

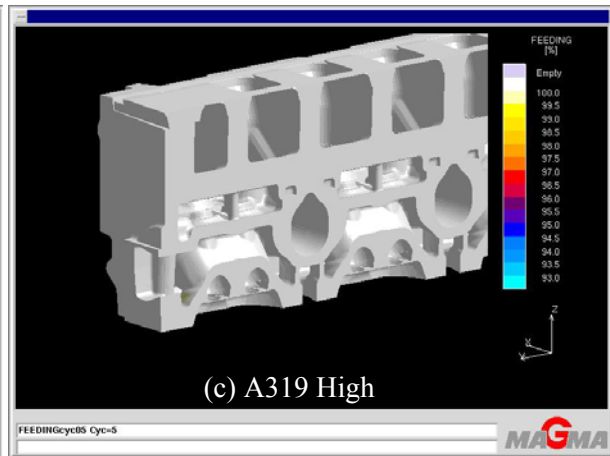
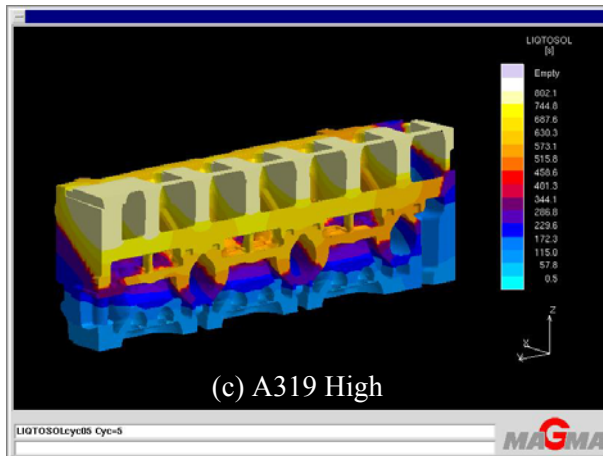
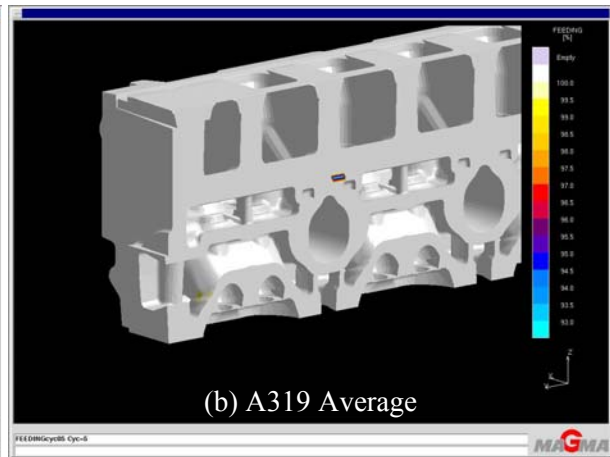
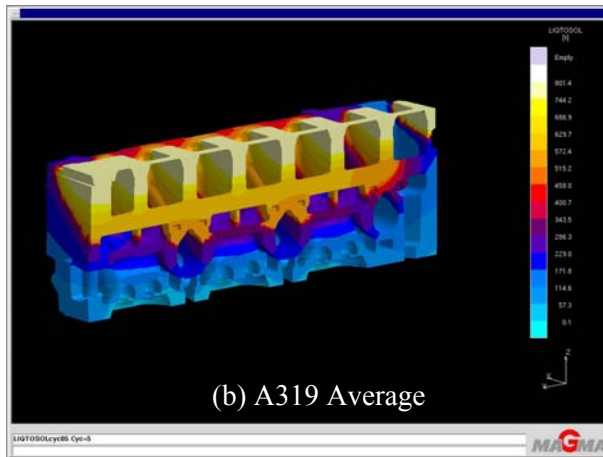
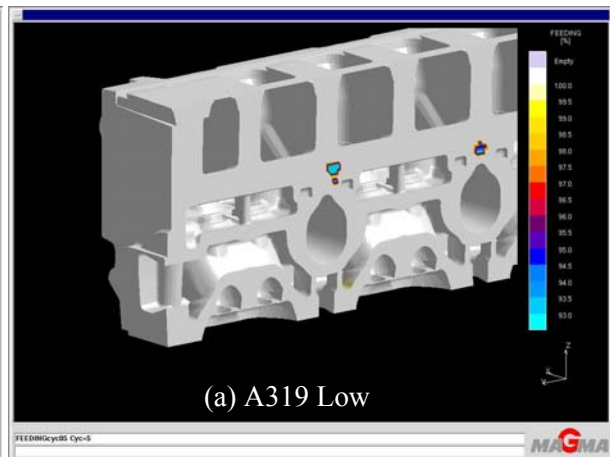
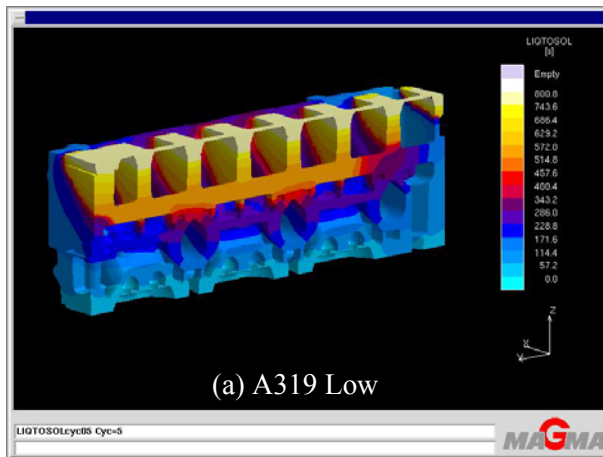


Figure 7. Calculated local solidification time for various A319 alloys

Figure 8. Calculated feeding/porosity for various A319 alloys

SUMMARY

The success in the recent development of computer software JMatPro for material property simulation has provided a reliable and cost-effective approach to generate the material data required by process simulation. The property data calculated by JMatPro has been used as direct inputs to casting simulation software MAGMASOFT®.

Two cases of casting have been studied. One for a cylinder head and the other for an aluminum step

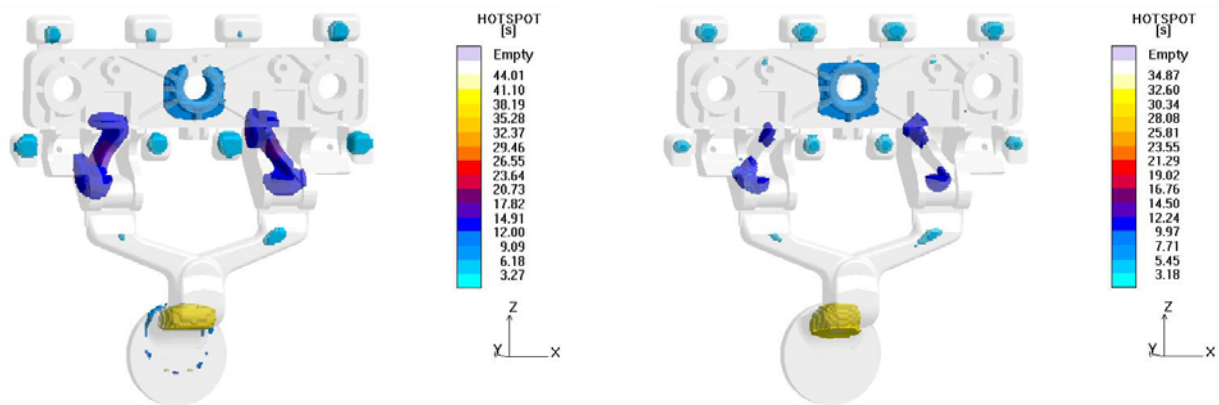


Figure 9. Comparison of calculated hotspots for casting of aluminium alloy A356 with higher (left) or lower (right) levels of Cu, Mn and Zn

for trucks. For the cylinder head, the overall effect of changing composition is significant. Core solidification behaviour is clearly changed and there is a substantial change in local solidification time as well as areas prone to hotspots and feeding behaviour. For the step casting, rather smaller changes in composition were utilised. In this case hot spot calculations clearly show a greater propensity for defect formation in the casting, indicating that impurity levels would have a significant effect on the soundness of the casting.

An advantage of using a calculation method is that the requisite material data can be rapidly calculated and the effect of varying the composition of an alloy within its specification range on a casting can be readily evaluated.

REFERENCES

1. <http://www.sentesoftware.co.uk/biblio.html>, A collection of free downloadable papers on the development and application of JMatPro, compiled by Sente Software Ltd., **2005**
2. N. Saunders, Z. Guo, X. Li, A.P. Miodownik and J-Ph. Schillé, *JOM*, December, **2003**, 60.
3. Z. Guo, N. Saunders, A.P. Miodownik and J.P. Schillé, *Materials Science and Engineering A*, **2005**, 413-414, 465-469.
4. N. Saunders, in *Solidification Processing 1997*, (Eds.: J. Beech and H. Jones), University of Sheffield, Sheffield, **1997**, 362.
5. N. Saunders, *Materials Science Forum*, **1996**, 217-222, 667.
6. N. Saunders, in *Light Metals 1997*, (Ed.: R. Huglen), TMS, Warrendale, PA, **1997**, 911.
7. R.A. Harding and N. Saunders, *American Foundrymen's Society Transactions*, **1997**, 105, 451.
8. B.A. Boutwell, R.G. Thompson, N. Saunders, S.K. Mannan, and J.J. deBarbadillo, in *Superalloys 718, 625, 706 and Various Derivatives*, (Ed.: E.A. Loria), TMS, Warrendale, PA, **1996**, 99.
9. Z. Guo, N. Saunders, A.P. Miodownik and J.P. Schillé, *Rare Metal Materials and Engineering*, **2006**, 35(Sup.1), 108-111.
10. E. Hepp, S. Neves, I. Egy, High precision measurement of thermophysical properties for liquid metals – Requirements for simulation of foundry processes, in *Modeling of Casting, Welding and Advanced Solidification Processes IX*, Eds.: P.R. Sahn, P.N. Hansen and J.G. Conley, Aachen, **2000**, 697-703.
11. S. Neves, Werkstoffdaten für die gießtechnische Simulation, in *Metall-Praxis*, **1-2/2002**, 752-755.