ARCHIVES of FOUNDRY ENGINEERING

Published quarterly as the organ of the Foundry Commission of the Polish Academy of Sciences

ISSN (1897-3310)
Volume 8
Issue 4/2008

157 – 162

29/4

3-D inverse solution for continuous casting taking an air cap into consideration

I. Nowak [a],*, J. Smołka [b], A. J. Nowak [b]

[a] Institute of Mathematics, Silesian University of Technology, Kaszubska 23, 44-100 Gliwice, Poland
[b] Institute of Thermal Technology, Silesian University of Technology, Konarskiego 22, 44-100 Gliwice, Poland
*Corresponding author. E-mail address: iwona.nowak@polsl.pl

Received 17.06.2008; accepted in revised form 08.07.2008

Abstract

The paper discusses a 3-D numerical solution of the inverse boundary problem for a continuous casting process of an aluminium alloy. Since the verified information on the heat flux distribution is crucial for a good design of a mould, effective cooling system and generally the whole caster, the main goal of the analysis presented within the paper was an identification of the heat fluxes along the external walls of the ingot. In the study an enthalpy-porosity technique implemented in a commercial Fluent package was used for modelling the solidification process. In this method, the phase change interface was determined on the basis of the liquid fraction approach. Moreover, the mathematical model included the pull velocity, the temperature-dependent properties for a liquid phase, mushy zone and solid phase, and a spatially local distribution of the thermal contact resistance between the ingot and crystallizer walls. In the inverse procedure, a sensitivity analysis was employed for the estimation of the boundary conditions retrieval. Although, the measured temperatures required to solve the problem are always burdened by measurement errors, a comparison of the measured and retrieved values showed a high accuracy of the computations.

Keywords: Application of information technology to the foundry industry, Boundary inverse problem, Sensitivity analysis

1. Introduction

In many branches of the contemporary industry quality of the casting material is very important. Since the continuous casting can satisfy many technical requirements, nowadays this technology is frequently utilized.

A possibility of the design as well as a control of the casting of metals, alloys, semiconductor crystals, etc. is very advisable. For this reason, numerical models may be successfully used to analyze some phenomena and processes in the continuous casting with relatively low costs.

The quality of the casting material is dependent on a procedure of cooling and a speed of the casting process. Therefore, a decision was made to reconstruct the cooling conditions in the continuous casting on the basis of measurements at some points inside the ingot. This kind of problems is formulated as the inverse boundary problem and in the presented work is solved employing a sensitivity analysis.

Similar problems were the subjects of the works dealing with both the boundary and the geometry inverse problems to estimate the geometry of a body [1]-[6]. However, a majority of them were formulated as two-dimensional problems and a number of model simplifications were assumed.

In this paper the heat flux distribution along the external boundary of 3-D model of ingot was estimated. In addition, the continuous casting of the aluminium alloy was considered. This resulted in modelling of mushy zones within computational domain. Moreover, a mathematical model included the momentum and the continuity equations apart from the energy equation. Such approach allowed one to analyze a natural convection in the liquid phase. In the mathematical description a thermal resistance along crystallizer was also taken into account. The thermal resistance between the ingot and crystallizer wall originates from a material contraction and is usually modelled as a constant value [7]. In this paper the thermal resistance is modelled as spatially local value determined on the basis of local temperatures of the ingot and crystallizer walls.

2. Problem formulation and direct problem

This section starts with a brief description of the mathematical model of the direct heat transfer problem for a continuous casting. The model serves as a basis for the inverse problem discussed in detail in the next section. The direct problem will also be employed to generate simulated temperature measurements for the application of the proposed inverse analysis algorithms.

The computational procedure of the unknown values retrieval was carried out iteratively and required the following main steps in each loop:

– a solution of the direct problem using a commercial Finite Volume Method code Fluent [8]. In the first iteration the unknown parameters i.e. boundary heat fluxes were assumed to be constant along the whole ingot and the temperature field inside the body was determined. The study showed that the developed procedures are effective even for different initial heat flux values comparing to the retrieved heat flux distribution. Moreover, the parameters as the under-relaxation factor and a number of iterations in each cycle were investigated to significantly decrease the computational time of the boundary retrieval computations.
– a solution of the inverse problem using an in-house code for the sensitivity analysis. Once the adequate objective function was minimized, the obtained values of heat fluxes were implemented into Fluent by User Defined Function (UDF) [8]. The mathematical model of the performed computations had to be supplemented with appropriate temperature measurements. The thermal inverse analysis discussed in the paper was based on the temperature measurements collected by thermocouples immersed in the liquid metal, carried by the cast and finally pulled out by the solidified ingot [3]-[4].

The geometrical model of the computational domain considered in the direct problem was in the shape of a brick with the following dimensions: 1.86 m x 0.51 m x 5.00 m, see Fig. 1. Due to two symmetry planes of the object, only one-fourth of it was analyzed. An influence of the numerical mesh generated within the geometry on the phase-change problem was investigated. Finally, the grid with almost 400 000 of hexahedral elements of very high quality was used in the inverse procedure.

The enthalpy-porosity technique was used in Fluent for modelling the phase change process [8],[10]. For this reason, the liquid fraction was computed at each iteration utilizing the enthalpy balance. For the solidification problem studied, the energy equation could be expressed as:

$$\nabla \cdot (k \nabla T) = \boldsymbol{\nabla} \cdot \rho \boldsymbol{w} H + \frac{\partial}{\partial t}(\rho H) \tag{1}$$

where k denotes the thermal conductivity, T stands for the temperature, ρ represents the density, $\boldsymbol{w}$ is the velocity vector, H denotes the enthalpy, and t is the time.

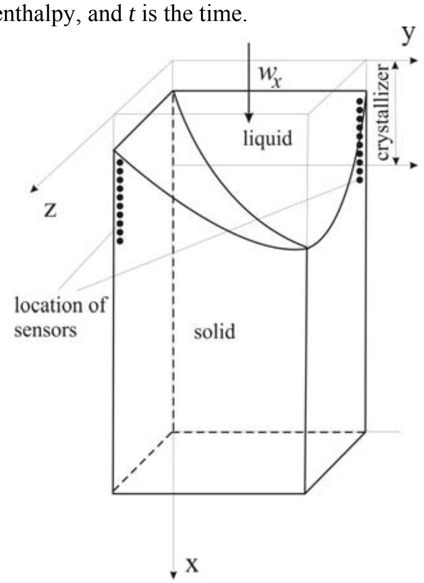

Fig. 1. Scheme of the 3-D computational domain of the continuous casting with locations of the temperature sensors

In the energy equation (Eq. (1)), the enthalpy of the material H was calculated as a sum of the sensible enthalpy and the latent heat:

$$H = h + \Delta H \tag{2}$$

where h is the sensible enthalpy, and ΔH represents the latent heat. The sensible enthalpy h can be determined on the basis of the following equation:

$$h = h_{ref} + \int_{T_{ref}}^{T} c_p dT \tag{3}$$

where h_{ref} denotes the reference enthalpy, T_{ref} is the reference temperature, and c_p stands for the specific heat at constant pressure.

The equation for the latent heat content ΔH can be written in terms of the latent heat of the material L:

$$\Delta H = \beta L \tag{4}$$

where β is the liquid fraction and takes the following values:

$$\begin{aligned} &\beta = 0 && \text{if} \quad T < T_S \\ &\beta = (T - T_S)/(T_L - T_S) && \text{if} \quad T_S \le T \le T_L \\ &\beta = 1 && \text{if} \quad T > T_L \end{aligned} \tag{5}$$

Apart from the energy equation, the mathematical model in the liquid phase included the momentum and the continuity equations to simulate the convective motions. Since the casting material was an alloy, the momentum equation was supplemented with additional source term describing a mushy zone region as a porous medium.

To solve the set of equations governing the casing process of alloys, appropriate material properties for the aluminium alloy and boundary conditions were defined.

As presented in Fig. 2, the thermophysical properties of the considered aluminium alloy are strongly dependent on temperature. Therefore, the density, the dynamic viscosity and the thermal conductivity were defined using polynomial functions of temperature for a liquid phase, mushy zone and solid phase. Since the temperature dependence of the specific heat is negligible, its value was assumed to be equal to 1170 J/(kgK). Moreover, the latent heat was set to 395 611 J/kg, while the solidus and liquidus temperatures were equal to 923.42 K and 838.15 K, respectively. As described above, latent heat content ΔH including the latent heat varied according to Eq. 4. between the solidus and liquidus temperatures. All material properties were determined using algorithms described in [11].

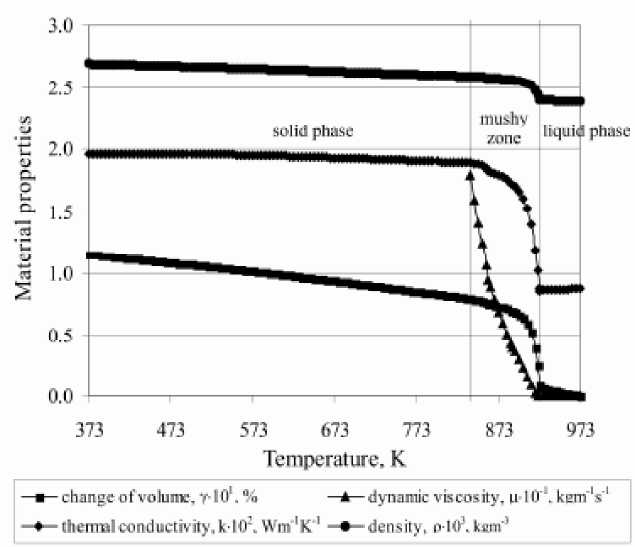

Fig. 2. Temperature-dependent material properties of the casted aluminium alloy

In the direct problem formulation the known boundary conditions were prescribed as in the real continuous casting process [3]. In such process the liquid material flows into a mould. Then inside the mould, the liquid material solidifies and is pulled out by withdrawal rolls along x-axis, see Fig. 1. For this reason, on the top surface of the computational domain, the velocity inlet boundary condition was defined with the following values: the inlet velocity was equal to the pull velocity $w_x = 0.001$ m/s, while the inlet temperature was equal to the liquid alloy temperature. Moreover, as already mentioned on two side walls of the model geometry, the symmetry boundary condition was prescribed.

The second group of boundary conditions consisted of the estimated heat flux profiles defined on the other two side surfaces of the body. The ingot is usually additionally cooled by water sprayed over the surface outside the crystallizer. A production technology of the continuous casting strongly depends on the heat flux distribution along the cooled boundaries of an ingot. On the basis of the subject literature and the published authors' papers [3], [5], [9], [12], it was assumed that the heat flux varied linearly along the mould and exponentially along the water spray. For this reason, only three heat fluxes needed to be estimated.

In this work the heat flux distribution was defined by functions dependent on three estimated fluxes q_1, q_2 and q_3 and variable x (casting was carried along this direction). The heat flux distributions were specified in the following form:

$$\begin{aligned}
-f_1(x) &= \frac{q_2-q_1}{d_m}\cdot x + q_1 \\
&\quad \text{if} \quad x \in < 0, d_m > \\
-f_2(x) &= \frac{q_3-q_2}{0.015}\cdot x + q_2 + \frac{q_3-q_2}{0.015}\cdot(d_m + 0.015) \\
&\quad \text{if} \quad x \in < d_m, d_m + 0.015 > \\
-f_3(x) &= q_3\cdot(0.85\cdot\exp(60\cdot(1.3-x)) + 0.621 - 0.465\cdot x) \\
&\quad \text{if} \quad x \geq d_m + 0.015
\end{aligned} \tag{6}$$

where d_m is the length of crystallizer, q_1 and q_2 are the values of the heat flux on the top and at the end of crystallizer, respectively. The variable q_3 indicates the heat flux at point just below the end of the mould.

At the points where casting body sinks the mould, the heat flux 'jump' appears. The linear function f_2 defining the heat flux distribution was assumed on a very short segment (its the length was equal to 0.015 m) under the end of the mould. Additionally, the exponential distribution of the heat flux was assumed on the part of the body that was cooled by sprayed water (function f_3).

In the problem presented the length of a crystallizer was 1 m which was approximately 20% of the solidified ingot length. The similar proportion of the ingot and the crystallizer lengths could be found in the literature [3].

During the solidification, a process of contraction occurs in both mushy zone and solid part of the ingot. A change of volume increases rapidly with the temperature drop, see Fig. 2. This strongly affects the cooling conditions. Therefore, to simulate a realistic casting process the thermal contact resistance was considered as well. This can be summarized as follows: for each grid cell, a geometrical volumetric contraction was determined using polynomial temperature dependent functions, see Fig. 2. Then the volumetric contraction was used to calculate an air gap between two cooled side wall of the ingot and internal walls of the crystallizer. As a result, spatially local values of contraction distribution were obtained. The heat is transferred through the air gap by radiation and also natural convection. Therefore, a final distribution of the thermal contact resistance was computed as a sum of the inverse of the radiative and convective heat transfer coefficients. The radiative heat transfer coefficient was determined based on the radiative heat exchange between two vertical walls, while the convective heat transfer coefficient was computed using formulas for the Nusselt equations for the closed rectangular enclosures. Both these procedures are well known in the heat transfer literature. It is worth mentioning that the temperatures occurring in those algorithms were local temperatures of the boundary cell centres and boundary cell faces. The thermal contact resistivity distribution is presented in Fig. 3

and is defined as thermal contact resistance multiplied by the solid fraction and divided by the cell height of the wall-adjacent cell.

The computations of the solidification process using the default parameters in Fluent turned out to be numerically unstable and led to disconvergence. For this reason, the direct problem was solved under unsteady conditions that significantly improved the stability of the iteration process. The time step size was increased gradually during calculations and its maximum value was equal to $\Delta t = 2$ s. The most effective inverse procedure was performed for the following parameters of the direct problem calculations in the iterative loop: the number of iterations in each time step equal to 10 and the number of time steps equal to 15. The final liquid fraction field obtained after boundary heat flux retrieval is illustrated in Fig. 4.

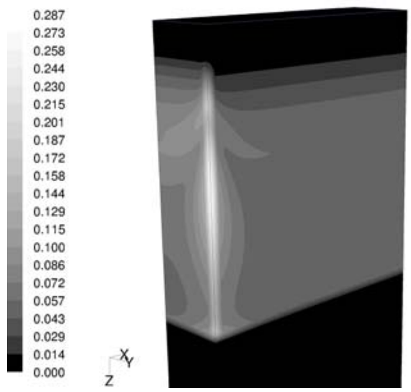

Fig. 3. The thermal contact resistivity in two cooled ingot walls

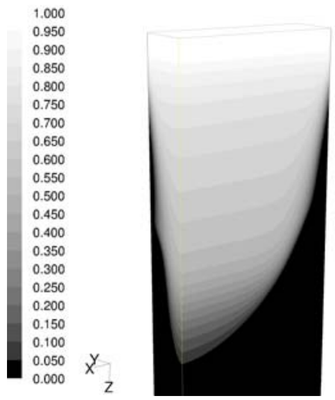

Fig. 4. The liquid fraction distribution in the casted material in two symmetrical planes

3. Formulation of the inverse boundary problem

A mathematical formulation of the boundary inverse thermal problem is very similar to the formulation of direct problems and consists of:

– a main equation describing phenomena under consideration,
– boundary conditions defining heat transfer processes along the boundary. One has to remember however, that for this kind of problem, some quantities occurring (usually collected in vector **Y**) are not known or at least uncertain.

This means that the mathematical description is incomplete and needs to be supplemented with the data collected during measurements. Typically, the temperatures U_i are measured at some points inside the ingot and collected in the vector **U**. On the other hand, it is very important to limit the number of sensors because of commonly known difficulties with the data acquisition. Moreover, apart form valuable information each measurement session introduces some noise as well.

In the presented inverse analysis, the estimation of the boundary conditions retrieval along the external surface of the ingot (3-D model) was performed. An application of Eq. (1) permits one to model the heat flux distribution using only three design variables, and as a result, it permits the reduction of the sensors number. Therefore, the objective was to estimate components of the vector **Y** which uniquely describes the reconstructed boundary conditions i.e heat flux distribution.

In the paper a concept of sensitivity coefficients was utilized in the procedure applied to find the solution of the discussed inverse heat transfer problem [3]. The coefficients **Z** are derivatives of the measured quantity i.e. temperature T_i at certain location, with respect to the assumed and then identified input data Yj [13]:

$$Z_{ij} = \frac{\partial T_i}{\partial Y_j} \tag{7}$$

The sensitivity coefficients can be calculated using different techniques. Its treatment as a solution of the adjoined boundary problem obtained by differentiation of thermal problem is one of the most effective. In the problem discussed the sensitivity coefficients resulted in three systems of equations that was equal to the number of estimated heat fluxes [4], [13].

It should be stressed that in the computations of the sensitivity coefficients the domain included the solidified part of the ingot only. As a result, the direct sensitivity problem is formulated on the basis of the heat conduction equation in the following form:

$$\nabla \cdot (k \nabla Z) = \boldsymbol{\nabla} \cdot \rho \boldsymbol{w} c_p Z + \frac{\partial}{\partial t}(\rho c_p Z) \tag{8}$$

while the boundary conditions along the external boundary (for ith design variable) equals:

$$\begin{aligned} -z_{1,i}(x) &= \tfrac{\partial}{\partial q_i}(f_1(x)) \quad \text{if} \quad x \in < 0, d_m > \\ -z_{2,i}(x) &= \tfrac{\partial}{\partial q_i}(f_2(x)) \quad \text{if} \quad x \in < d_m, d_m + 0.015 > \\ -z_{3,i}(x) &= \tfrac{\partial}{\partial q_i}(f_3(x)) \quad \text{if} \quad x \geq d_m + 0.015 \end{aligned} \tag{9}$$

The remainder of the defined boundary conditions on the top, bottom and the symmetry planes of the body were maintained as in the original thermal problem.

The obtained sensitivity coefficients provided a measure of each identified value and indicated how the searched values are modified in the retrieval process. Additionally, the coefficients determined the locations of the most precise temperature sensors.

The ill-posed nature of the inverse problem causes that a number of temperature sensors should be appropriate to make the problem over determined. It means that a number of measurements needs to be bigger than a number of the unknown values. In consequence, the inverse analysis leads to optimization procedures with least squares calculations of the objective functions Δ (the goal is to minimize the difference between measured **U** and calculated temperatures $\mathbf{T}_{cal}$). However, in some cases (also studied here), an additional term should be used to improve stability [4], [9], i.e.:

$$\Delta = (\mathbf{T}_{cal} - \mathbf{U})^T \mathbf{W}^{-1} (\mathbf{T}_{cal} - \mathbf{U}) + \\ + (\mathbf{Y} - \mathbf{Y}_E)^T \mathbf{W}_Y^{-1} (\mathbf{Y} - \mathbf{Y}_E) \rightarrow \min \qquad (10)$$

Using the sensitivity analysis and some basic algebraic manipulations, a minimization of the objective function leads to the following set of equations [4]-[5]:

$$(\mathbf{Z}^T\mathbf{W}^{-1}\mathbf{Z} + \mathbf{W}_Y^{-1})\mathbf{Y} = \\ = \mathbf{Z}^T\mathbf{W}^{-1}(\mathbf{U} - \mathbf{T}^*) + (\mathbf{Z}^T\mathbf{W}^{-1}\mathbf{Z})\mathbf{Y}^* + \mathbf{W}_Y^{-1}\mathbf{Y}_E \qquad (11)$$

where the vector **T*** contains the temperatures calculated at temperature sensor locations, **U** stands for the vector of the temperature measurements and superscript T denotes the transpose matrices. Symbol **W** refers to the covariance matrix of measurements. This is a diagonal matrix with the values of an error in an adequate location on diagonal. Thus, the contribution of more accurately measured data is stronger than those obtained with lower accuracy. The unknown variables are collected in the vector **Y**, while the known prior estimates in the vector $\mathbf{Y}_E$. The symbol $\mathbf{W}_Y$ stands for the covariance matrix of the prior estimates. It means that on a diagonal of matrix $\mathbf{W}_Y$ there are the estimated errors of the identified values.

This procedure was successfully applied for both boundary and geometry inverse problems in 2-D model [5]. For this reason, it was decided to use the above algorithm in 3-D case. For this kind of formulation, the inverse problem is solved by building up a series of direct solutions, which gradually approaches the correct values of the design variables. The single iteration was realized in two steps. In the first, the mathematical description of the thermal process was completed by assuming the arbitrary, but known values collected in vector $\mathbf{Y}_E$. In consequence the problem can be solved as the direct one. In the second step, temperatures obtained in the solved direct problem were compared with measured values **U** and then the assumed data $\mathbf{Y}_E$ were modified.

As mentioned in the previous section, in a particular cycle the solution was only partly converged (15 times steps, and 10 iterations per time step). This means that the final values of the retrieved heat fluxes were obtained after a number of the cycles.

4. Numerical calculations and results

The assumptions reported in section 2 resulted in a vector of the estimated variables containing three components i.e. $\mathbf{q} = [q_1, q_2, q_3]$. In the numerical model the heat fluxes had the following values: q_1 = -0.5 MW/m^2, q_2 = 0 W/m^2, q_3 = - 1.9 MW/m^2, and for these values, the temperatures at sensor points were calculated.

Since the experimental tests are always burdened with errors, the numerically simulated measurements were modified by adding the random errors with a uniform distribution to the temperatures at the sensor points. It should also be stressed that the inverse problem is always ill-posed. As a consequence, the estimated heat fluxes might be very inaccurate. For this reason, an influence of the measurement accuracy on the quality of heat fluxes estimation is discussed in the paper.

The assumed measurement errors did not exceed 5% i.e. the errors equal to 0.1%, 0.2%, 1% , 2% and 5% were considered. In addition, the calculations with "error" equal to 0% were carried out to test the procedure. All obtained results are presented in Table 1.

Table 1.
Numerical results

	Measurement error in %	Estimated value in W/m^2	Average error in sensor points in K (in %)
q_1	0.0	-500 265	0.00671 (0.00086)
q_2		78	
q_3		-1 899 583	
q_1	0.1	-500 077	0.27591 (0.03798)
q_2		113	
q_3		-1 897 627	
q_1	0.2	-500 536	0.59437 (0.07597)
q_2		103	
q_3		-1 895 336	
q_1	1.0	- 501 089	2.98192 (0.38086)
q_2		515	
q_3		-1 878 917	
q_1	2.0	- 501 872	5.96017 (0.76049)
q_2		938	
q_3		-1 858 500	
q_1	5.0	- 504 640	14.89452 (1.8948)
q_2		2 182	
q_3		-1 796 991	

In the real problems a comparison of the measurements and the temperatures calculated in the model is the only possibility. The average error presented in last column of Table 1 should be understood as the arithmetic mean of the error in all sensor points. The absolute difference between the temperatures calculated at sensor points and obtained from measurement was the error in K, while the average percentage error was calculated as the averaging quotient of the absolute difference mentioned.

Fig. 5 presents a comparison of the temperatures at sensor locations calculated in the direct, fully liquid-solid model (taking an air gap into consideration), numerically simulated measurements (with errors not bigger than 2%), and the temperatures calculated for the retrieved boundary conditions in the inverse procedure.

It should be stressed that for different error levels the obtained results demonstrated similar accuracy and in all cases the stabilization of iteration process was observed after 80-100 iterations.

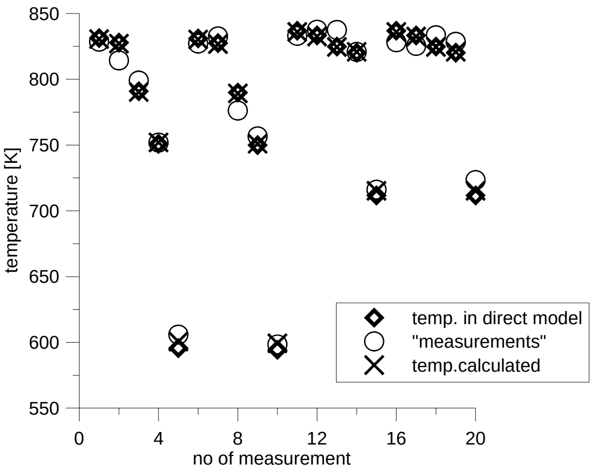

Fig. 5. The temperature values at sensor locations obtained in the iteration procedure

5. Conclusions

This paper discussed an identification procedure of the heat flux distribution along an ingot external boundary in continuous casting. The problem was formulated as a 3-D inverse boundary problem and was solved as a series of direct solutions, which gradually produced very accurate values of the designed variables. The proposed algorithm was a generalization of the method developed for 2-D problems. In order to limit the number of retrieved values, the heat flux distribution was approximated. It considerably allowed the reduction of a number of the estimated values.

Acknowledgements

The financial assistance of the Ministry of Science and Higher Education, Poland, grant No. 3 T10B 007 30 is gratefully acknowledged herewith.

References

[1] E. Majchrzak, J. Mendakiewicz, Identification of cast iron substitute thermal capacity, Archiwum Odlewnictwa, vol. 6 (2006) 310-315

[2] B. Mochnacki, E. Pawlak, J. S. Suchy, Identification of alloy latent heat on the basis of mould temperature (part 2), Archives of Foundry, vol. 6 (2006) 331-337.

[3] J.-M. Drezet, M. Rappaz, G. -U. Grun, M. Gremaud, Determination of Thermophysical Properties and Boundary Conditions of Direct Chill-Calst Aluminium Alloys Using Inverse Methods, Metallurgy And Materials Transactions, vol. 31 (2000) 1627-1634.

[4] A. J. Nowak, BEM Approach to Inverse Thermal Problems, Chapter 10 in D. B. Ingham, L. C. Wrobel, Boundary Integral Formulations for Inverse Analysis, Computational Mechanics Publications, Southampton (1997).

[5] I. Nowak, A. J. Nowak, L. C. Wrobel, Tracking of Phase Change Front for Continuous Casting - Inverse BEM Solution, in Inverse Problems in Engineering Mechanics II, Proceedings of ISIP 2000, Nagano, Japan (2000) 71-80.

[6] R. Conde, M. T. Parra, F. Castro, J. M. Villafruella, M. A. Rodriguez, C. Mendez, Numerical model for two-phase solidification problem in a pipe, Applied Thermal Engineering, vol. 24 (2004) 2501-2509.

[7] T. A. Blase, Z. X. Guo, Z. Shia, K. Long, W. G. Hopkins, 3D conjugate heat transfer model for continuous wire casting, Materials Science and Engineering, vol. 365 (2004) 318-324.

[8] Fluent Product Documentation, www.fluent.com.

[9] K. Kurpisz, A. J. Nowak, Inverse Thermal Problems, Computational Mechanics Publications, Southampton, 1995.

[10] V. R. Voller, C. Prakash, A Fixed-Grid Numerical Modelling Methodology for Convection-Diffusion Mushy Region Phase-Change Problems, International Journal of Heat Mass Transfer vol. 30 (1987) 1709-1720.

[11] Z. Guoa, N. Saunders, A. P. Miodownik, J. -P. Schille, Modelling of materials properties and behaviour critical to casting simulation, Materials Science and Engineering, vol. 413 (2005) 465-469.

[12] I. Nowak, J. Smołka, A. J. Nowak, Effective inverse procedure for retrieving boundary condition in three-dimensional continuous casting problem, Proceedings of the International conference on the Inverse Problems in Engineering, Paris, 2008.

[13] J. V. Beck, B. Blackwell, Inverse Problem, in W. J. Minkowycz, E. M. Sparrow, G. E. Schneider, R. H. Pletcher, Handbook of Numerical Heat Transfer, Wiley, New York (1988).