

# Reconstruction of the heat transfer coefficient on the grounds of experimental data

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Received 22.01.2009; published in revised form 01.05.2009

## Analysis and modelling

### ABSTRACT

**Purpose:** Solidification of pure metal can be modelled by a two-phase Stefan problem, in which the distribution of temperature in the solid and liquid phases is described by the heat conduction equation with initial and boundary conditions. The inverse Stefan problem can be applied to solve design problems in casting process.

**Design/methodology/approach:** In numerical calculations the alternating phase truncation method, the Tikhonov regularization and the genetic algorithm were used. The featured examples of calculations show a very good approximation of the experimental data.

**Findings:** The verification of the method of reconstructing the cooling conditions during the solidification of pure metals. The solution of the problem consists of selecting the heat transfer coefficient on the boundary, so that the temperature in selected points on the boundary of the domain assumes given values.

**Research limitations/implications:** The method requires that it must be possible to describe the sought boundary condition by means of a finite number of parameters. It is not necessary, that the sought boundary condition should be linearly dependent on those parameters.

**Practical implications:** The presented method can be easily applied to solve design problems of different types, e.g. for the design of continuous casting installations (incl. the selection of the length of secondary cooling zones, the number of jets installed in individual zones, etc.).

**Originality/value:** Verification, on the grounds of experimental data, the formerly devised method of determining the heat transfer coefficient during the solidification of pure metals.

**Keywords:** Artificial intelligence methods; Casting; Inverse Stefan Problem

#### Reference to this paper should be given in the following way:

D. Słota, Reconstruction of the heat transfer coefficient on the grounds of experimental data, Journal of Achievements in Materials and Manufacturing Engineering 34/1 (2009) 63-70.

## 1. Introduction

The inverse problem provides a very useful tool for analyses of heat transfer processes, including solidification processes [1,2]. In the case of inverse problems the causes of the described phenomena are unknown, or are not fully determined. The unique solutions of

such problems require additional information, for example, temperature measurements at selected points of the domain.

The Stefan problem poses an interesting case of heat transfer processes, involving mathematical models describing heat processes characterized by the phase changes and the resultant emission and absorption of heat. These processes include: solidification of metals, formation of crystals, formation of

igneous rock, food refrigeration, freezing of soil and water, ice melting, etc. The Stefan problem entails a simultaneous determination of the distribution of temperature in the domain and the location of the boundary separating the domain into the sub-domains of the liquid and solid phase.

It is commonly assumed in the discussion of the inverse Stefan problem that the additional information compensating the absence of input data is some knowledge of the location of the boundary of the phase change, its velocity in the normal direction or temperature at selected points of the domain. Actually, the problems for which the additional information specifies the location of the phase change boundary are often regarded as design problems.

Both in the inverse heat conduction problems and in the inverse Stefan problems the following tasks may be considered: initial values (retrospective), boundary values, parametric values (coefficients). The above mentioned problems are ill-posed, i.e. the solution of the problem may not exist, or, if it exists, it may be non-unique or unstable. Therefore, it is difficult to select an appropriate method of obtaining solutions or theoretical results. Thus, so far there have been few publications concerning the inverse Stefan problem, especially in comparison with works focused on the direct Stefan problem. Only one monograph dedicated to the discussion of this issue has been published [3].

The two-phase one-dimensional inverse Stefan problem in which it is necessary to designate the function for the formulation of the boundary conditions of the second kind was discussed in [4], where the author stipulated the conditions for the existence, uniqueness and the linear dependence of the solution on the initial data. The approximated solution is derived in the course of the iteration of the integral equations containing Green's functions and Neumann's functions for Laplace equation.

Whereas, in [5,6] the mollification method for one-phase, one-dimensional inverse Stefan problem, involving the reconstruction of temperature and heat flux on the boundary of the domain with given location of the phase change front, was discussed.

Furthermore, in [7] the heat flux on the boundary of the domain was determined if the velocity of the phase change front and the heat fluxes permeating it were known. The task was simplified to the minimization of the functional constructed with the use of sensitivity coefficients. Accordingly, in [8] two methods of the solution of the above mentioned task were presented. Both of the methods employed the minimization of the square error in view of the calculated and given temperature of the phase change front (for the entire time section). The first method used the spline functions approximation of an unknown heat flux, i.e. the minimization was conducted in finitely dimensional space. In the second method the minimization of the functional cost was conducted by means of finite conjugate gradients or steepest descend (saddle-point) methods. The same problem for the two-dimensional case was discussed in [9]. In [10] the inverse problem was investigated in the domain, where in the liquid phase the heat transfer took place by conduction and convection. The problem was divided into two independent solutions. The first one was a direct convection task in the liquid phase; the second was the inverse task in the solid phase. Whereas, in [11] both component tasks were regarded as inverse problems. Similar issues were also considered in [1,12-14].

In [15] the heat balance integral method was applied to solve the inverse Stefan problem. The author assumed that the temperature distribution in the solid phase was described by the third degree polynomial. One-phase and two-phase one-dimensional problem, for which the function describing the boundary condition must be designated, was considered.

In [16,17] Adomian decomposition method and the variational iteration method in conjunction with optimization to the approximate solution of one-phase inverse Stefan problem were discussed. Conversely, in [18-20] the same authors applied the optimization or approximation method to solve the two-phase or three-phase design problem for a one-dimensional or two-dimensional case.

In view of an increasing popularity of genetic algorithms, they have also had a wide application for solving the inverse problems, for example in [21], or in [22-25] where the method of solving the inverse Stefan problem is based on genetic algorithms. The solution consists in selecting the heat transfer coefficient (or heat flux) on one of the boundaries in such a way that the phase change front accepts the assumed location, or that the temperature calculated at selected points of the domain approximates the given values as exactly as possible. The method has been stable both in terms of errors in the initial data, as well as the number of control points; moreover, it is more exact in comparison with the methods based on classic optimization algorithms.

There are also other papers available, which deal with various problems connected with solidification or heat treatment of different materials (see for example [26-31]).

In this paper the method of reconstructing the function describing the boundary conditions in the solidification of aluminium is verified on the grounds of experimental data. An algorithm enabling the solution of the inverse Stefan problem, where additional information consists of temperature measurements at selected points of the domain, is presented. The calculations use the experimental data obtained in the course of aluminium solidification process. Based on given information about the temperature measurements, a functional defining the error of an approximate solution is constructed. To find the minimum of the functional, a genetic algorithm is used [32,33]. For the solution of a direct Stefan problem, the alternating phase truncation method is applied [23,34].

## 2. Governing equations

The boundary of the considered domain (see Figure 1):

$$D = [0, b] \times [0, t^*] \subseteq R^2 \quad (1)$$

will be divided into three parts:

$$\Gamma_0 = \{(x, 0), \quad x \in [0, b]\}, \quad (2)$$

$$\Gamma_1 = \{(0, t), \quad t \in [0, t^*]\}, \quad (3)$$

$$\Gamma_2 = \{(b, t), \quad t \in [0, t^*]\}, \quad (4)$$

for which an initial condition and boundary conditions are defined. Let  $D_1$  denote the subset of domain  $D$ , which is occupied by a liquid phase, and let  $D_2$  denote the domain occupied by a solid phase. The moving interface (freezing front)

will be denoted as  $\Gamma_g$ . Let us assume that it is described by function  $x = \xi(t)$ .

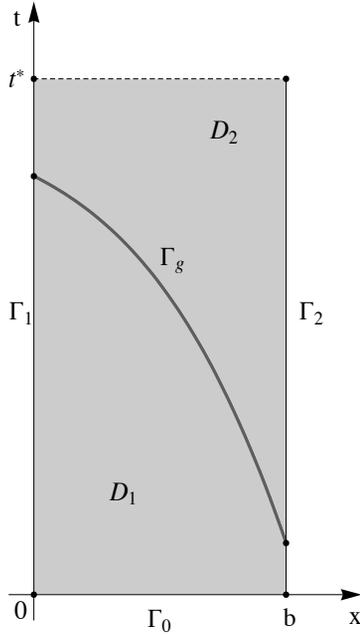


Fig. 1. Domain of the problem

In the discussion the cooling conditions in the process are selected in such a manner that the temperature at given points of the domain will have the following values:

$$T_2(r_i) = U_i, \quad i = 1, 2, \dots, N, \quad (5)$$

where  $r_i \in D$ , and  $N$  denotes the number of the measurements. Furthermore, we designate the position of the freezing front  $\Gamma_g$  and the temperature distributions  $T_k$  in domains  $D_k$  ( $k = 1, 2$ ), which fulfil the heat conduction equation ( $(x, t) \in D_k$ ):

$$c_k \rho_k \frac{\partial T_k}{\partial t}(x, t) = \frac{1}{x} \frac{\partial}{\partial x} \left( \lambda_k x \frac{\partial T_k}{\partial x}(x, t) \right), \quad (6)$$

where  $c_k$ ,  $\rho_k$  and  $\lambda_k$  are the specific heat, the mass density and the thermal conductivity in the liquid phase ( $k = 1$ ) and solid phase ( $k = 2$ ), respectively. On the boundary  $\Gamma_0$  the initial condition is determined ( $T_0 > T^*$ ):

$$T_1(x, 0) = T_0. \quad (7)$$

On the boundary  $\Gamma_1$  a homogeneous boundary condition of the second kind is designated:

$$\frac{\partial T_k}{\partial n}(0, t) = 0. \quad (8)$$

On the boundary  $\Gamma_2$  the boundary condition of the third kind is designated:

$$-\lambda_k \frac{\partial T_k}{\partial n}(b, t) = \alpha(t)(T_k(b, t) - T_\infty), \quad (9)$$

where  $\alpha$  is the heat transfer coefficient and  $T_\infty$  is the surrounding temperature. Whereas, on the freezing front  $\Gamma_g$  the temperature continuity condition and the Stefan condition are designated:

$$T_1(\xi(t), t) = T_2(\xi(t), t) = T^*, \quad (10)$$

$$-\lambda_1 \frac{\partial T_1(\xi(t), t)}{\partial x} + \lambda_2 \frac{\partial T_2(\xi(t), t)}{\partial x} = L \rho_2 \frac{d\xi(t)}{dt}, \quad (11)$$

where  $T^*$  is the temperature of melting point,  $L$  is the latent heat of solidification.

Function  $\alpha(t)$ , describing the heat transfer coefficient, will be sought in the form of a function dependent (in a linear or non-linear way) on  $n$  parameters:

$$\alpha(t) = \alpha(t; \alpha_1, \alpha_2, \dots, \alpha_n). \quad (12)$$

Let  $V$  denotes a set of all functions in the form of (12). In real processes, function  $\alpha(t)$  does not have an arbitrary value. Therefore, the problem of minimization with constraints has some practical importance. Assuming that:

$$V_\alpha = \{ \alpha(t) \in V, \quad \alpha_i \in [\alpha_i^l, \alpha_i^u], \quad i = 1, 2, \dots, n \}. \quad (13)$$

For the determined function  $\alpha(t) \in V_\alpha$ , the problem (6)-(11) becomes a direct Stefan problem, the solution of which allows to find the courses of temperatures  $T_i = T_2(r_i)$  corresponding to function  $\alpha(t)$ . Using the calculated temperatures  $T_i$  and the given temperatures  $U_i$ , we can build a functional which will determine the error of the approximate solution:

$$J(\alpha) = \sum_{i=1}^N (T_i - U_i)^2. \quad (14)$$

### 3. Genetic algorithm

To find the minimum of the functional (14), a genetic algorithm was used [32,33]. In the calculations real number representation of a chromosome and a tournament selection was used. This selection was carried out in such a manner that two chromosomes were drawn and the one with better fitness went to a new generation. There were so many draws as many individuals the new generation was supposed to include. An elitist model was also applied in the algorithm, where the best individual of the previous generation is saved and, if all individuals in the current generation are worse, the worst of them is replaced with the best individual from the previous population.

As the crossover operator, the arithmetical crossover was applied, where as a result of the crossing of chromosomes  $\alpha^1 = (\alpha_1^1, \alpha_2^1, \dots, \alpha_n^1)$  and  $\alpha^2 = (\alpha_1^2, \alpha_2^2, \dots, \alpha_n^2)$ , their linear combinations were obtained:

$$\alpha^1 = p\alpha^1 + (1-p)\alpha^2, \quad (15)$$

$$\alpha^2 = p\alpha^2 + (1-p)\alpha^1, \quad (16)$$

where parameter  $p$  is a random number with a uniform distribution from the domain  $[0,1]$ . In the calculations, a nonuniform mutation operator was used as well. During mutation, the  $\alpha_i$  gene from chromosome  $\alpha = (\alpha_1, \dots, \alpha_i, \dots, \alpha_n)$ , was transformed according to the equation:

$$\alpha_i' = \begin{cases} \alpha_i + \Delta(\tau, \alpha_i^u - \alpha_i), \\ \alpha_i - \Delta(\tau, \alpha_i - \alpha_i^l), \end{cases} \quad (17)$$

and a decision about which one from the above formulas should be applied was taken at random. Function  $\Delta(\tau, \alpha)$  was assumed in the form:

$$\Delta(\tau, \alpha) = \alpha(1 - p^{(1-\tau/M)^g}), \quad (18)$$

where  $p$  is a random number with a uniform distribution from the domain  $[0,1]$ ,  $\tau$  is a current generation number,  $M$  is a maximum number of generations and  $g$  is a constant parameter (in the calculations,  $g = 2$  was assumed).

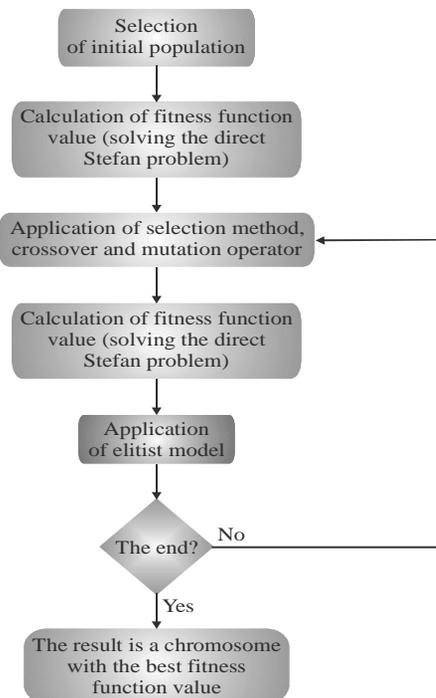


Fig. 2. Flowchart of the genetic algorithm

The flowchart of the genetic algorithm was shown in Figure 2. In the calculations the parameters used for the genetic algorithm are as follows:

- population size  $n_{pop} = 70$ ,
- number of generations  $M = 100$ ,

- crossover probability  $p_c = 0.7$ ,
- mutation probability  $p_m = 0.1$ .

#### 4. Alternating phase truncation method

To solve a direct Stefan problem, the alternating phase truncation method was applied [23,34]. In this method in place of temperature we insert an enthalpy:

$$H(T) = \int_0^T c(s)\rho(s)ds + \eta(T)L\rho_2, \quad (19)$$

where

$$\eta(T) = \begin{cases} 1 & \text{for } T > T^*, \\ 0 & \text{for } T \leq T^*. \end{cases} \quad (20)$$

Function  $H(T)$  is discontinuous in the point given by the temperature of the phase change  $T^*$ . Its left-hand and right-hand limits at this point will be denoted as  $H_s$  and  $H_l$ :

$$H_s = \int_0^{T^*} c(s)\rho(s)ds, \quad (21)$$

$$H_l = H_s + L\rho_2. \quad (22)$$

If we use equation (19) in the Stefan problem, we will obtain in both phases, a heat conduction equation where the temperature will be replaced with enthalpy.

The algorithm of the alternating phase truncation method (for one time's step) consists of two stages. Let's assume that we know the distribution of enthalpy in time  $t_i$  from the initial condition or from the previous step of the calculations. In the first stage we reduce the entire domain to a liquid phase, i.e. to the points at which the value of the enthalpy is smaller than  $H_l$  and supply (symbolically) such quantity of heat that the enthalpy equals to  $H_l$ . The so obtained heat transfer problem in a one-phase domain can be solved by one of the known methods (e.g. the finite-difference method), thereby obtaining an approximate distribution of enthalpy. At points to which we have supplied a certain amount of heat, the same amount must be now deducted. After this operation we obtain the distribution of enthalpy, which is treated as a starting point for the second stage of calculations (at moment  $t_i$ ).

In the second stage, we reduce the whole domain to a solid phase, i.e. at those points of the domain where the enthalpy value is higher than  $H_s$ , we carry away (symbolically) such amount of heat that would allow the enthalpy to adopt a value equal  $H_s$ . Like in the first stage, we find an approximate distribution of enthalpy. At the end of the second stage, at the points where we artificially carried away a certain amount of heat, we add the same amount of heat. This completes the second stage and at the same time, one step of the calculations (transfer from time  $t_i$  to time  $t_{i+1}$ ) of the alternating phase truncation method.

In the alternating phase truncation method, for each time step, the heat transfer equation is solved twice. Therefore, we must see to appropriate consideration of the boundary conditions, so that they would influence the discussed system only over time  $\Delta t$ , and not  $2\Delta t$ . In the first stage of the alternating phase truncation method, we take the real boundary conditions only on those boundary fragments where the liquid phase contacts the neighborhood. At the same time, we isolate the remaining fragments of the boundary. In the second stage, we consider the real boundary conditions on those boundary fragments where the solid phase contacts the neighborhood and we isolate the remaining fragments of the boundary.

## 5. Calculations

The calculations are based on the experimental data obtained in the course of aluminium (EN AW-Al99.5) solidification process. The experiment was performed with the use of the Universal Metallurgical Stimulator and Analyzer (UMSA) - an instrument designed for the analysis of thermal processes of metal samples [35-38]. In the experiment, two cylinder samples with the diameter of 18 mm and height of 20 mm were used. The material was melted in a crucible induction furnace and cast into a graphite mould with the diameter of 25 mm. Next, it was mechanically treated to achieve the require dimensions. A thermocouple was mounted in a central part of sampling casting and connected to the recording device. Three complete melting and solidification loops of the sample were performed in the course of the experiment, that is: each sample rendered three temperature distributions.

The calculations are focused on reconstructing function  $\alpha$  dependent on a different number of parameters (one, three, six, ten or twenty):

$$\alpha(t) = \alpha(t; \alpha_1, \alpha_2, \dots, \alpha_n), \quad n \in \{1, 3, 6, 10, 20\}. \quad (23)$$

In the alternating phase truncation method, the finite-difference method was used. The calculations made on the grid of discretization intervals equalling  $\Delta t = 0.1$  and  $\Delta x = b/500$ .

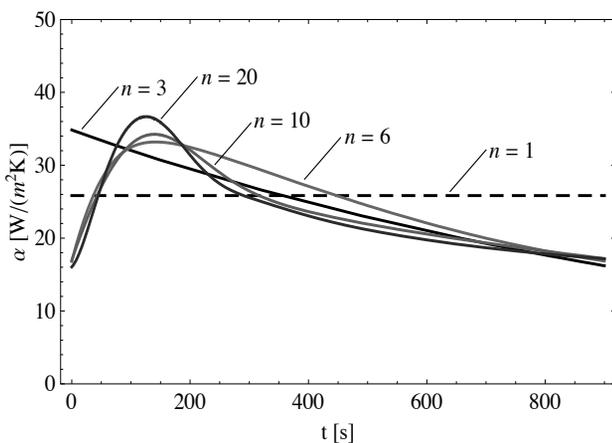


Fig. 3. The heat transfer coefficient reconstructed for a different number of parameters

In Figure 3 the heat transfer coefficient reconstructed for different number of the sought parameters is shown; whereas Figures 4, 5 and 6 present the cooling curve plotted in the course of the experiment and its reconstruction for the designated heat transfer coefficient. Absolute errors of the reconstruction of the cooling curve are shown in Figures 7, 8 and 9. The mean and maximal relative and absolute errors of the reconstruction of the cooling curve for the heat transfer coefficient derived for different number of the sought parameters are compiled in Table 1.

Table 1.

Errors in the reconstruction of the cooling curve ( $\delta_{mean}$  - mean relative percentage error,  $\delta_{max}$  - maximal relative percentage error,

$n$	1	3	6	10	20
$\delta_{mean}$ [%]	4.840	0.559	0.341	0.227	0.232
$\delta_{max}$ [%]	10.538	4.207	1.907	1.469	1.433
$\Delta_{mean}$ [K]	27.836	3.939	2.436	1.520	1.450
$\Delta_{max}$ [K]	68.910	40.974	17.460	13.510	13.180

The results indicate that an increase in the number of the parameters leads to a better reconstruction of the cooling curve. At the same time, the mean and maximal values of relative and absolute errors decrease. The only exception is the case of ten parameters, for which the mean relative percentage error is 0.227 % and is insignificantly smaller than the corresponding error for twenty parameters (which equals 0.232 %). Such result may have been caused by the fact that the biggest errors for ten parameters occurred at the points of higher temperature as compared with the case of twenty parameters. All the other errors for twenty parameters are smaller than the corresponding errors for the case of ten parameters.

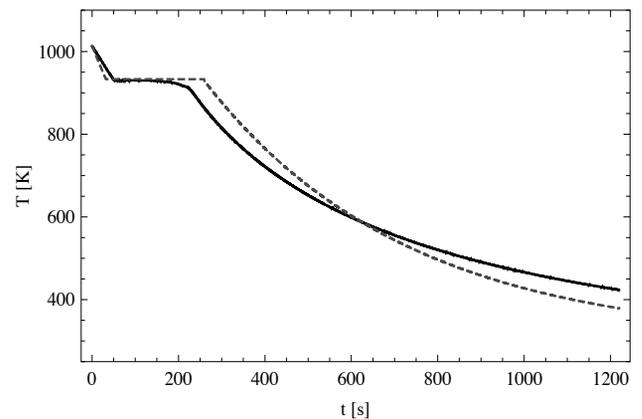


Fig. 4. The cooling curve (solid line - measurement data, dashed line - the curve reconstructed for one parameter)

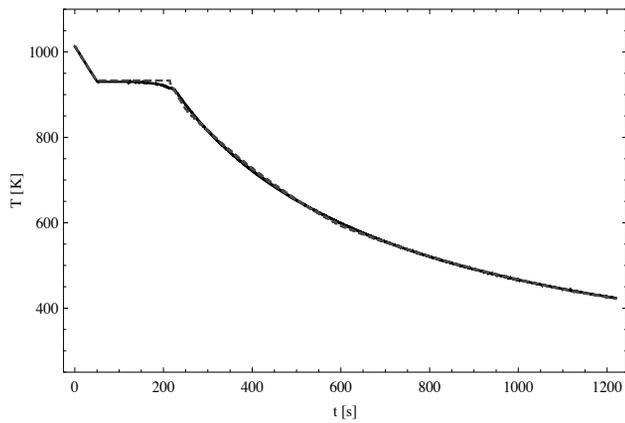


Fig. 5. The cooling curve (solid line - measurement data, dashed line - the curve reconstructed for six parameters)

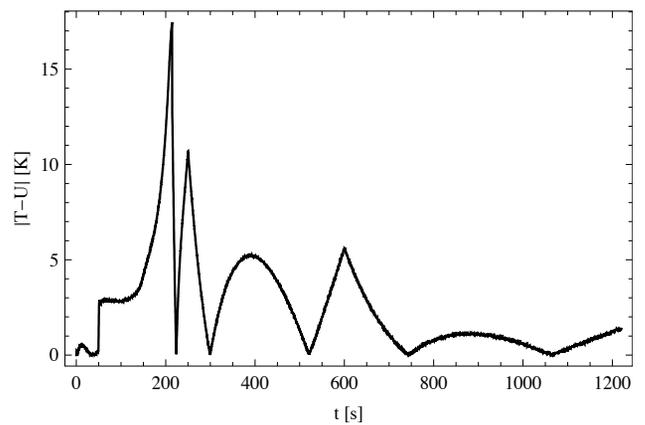


Fig. 8. The absolute errors of the reconstruction of the cooling curve for six parameters

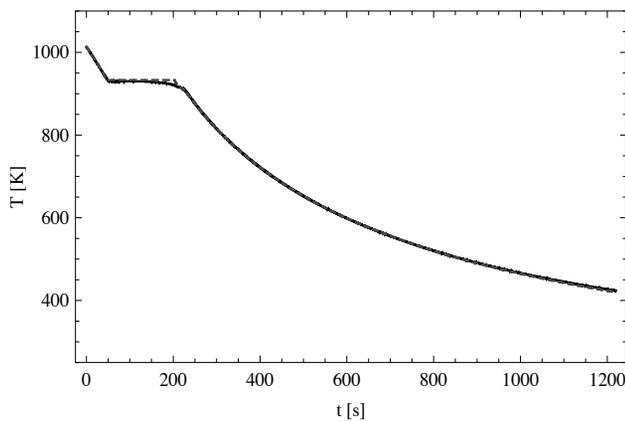


Fig. 6. The cooling curve (solid line - measurement data, dashed line - the curve reconstructed for twenty parameters)

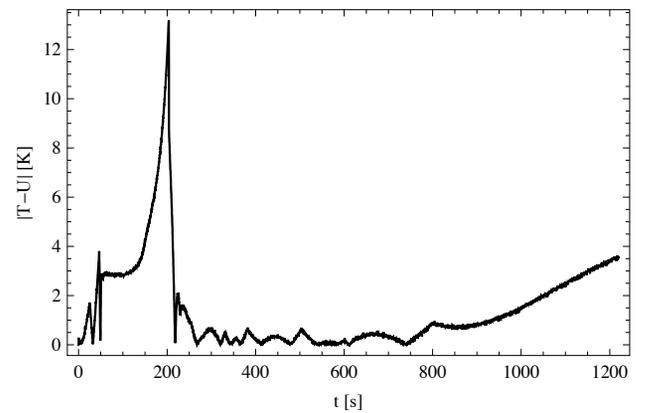


Fig. 9. The absolute errors of the reconstruction of the cooling curve for twenty parameters

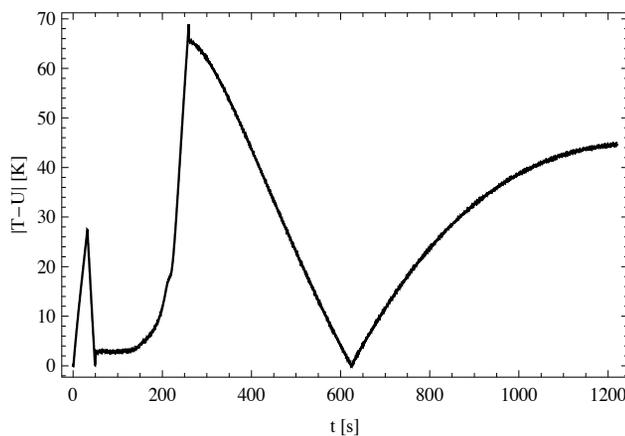


Fig. 7. The absolute errors of the reconstruction of the cooling curve for one parameter

## 6. Conclusions

In the paper, on the grounds of the cooling curves designated in the course of the solidification of aluminium, the heat transfer coefficient on the boundary of the domain was derived. The process was modelled on the one-dimensional inverse Stefan problem. The results indicate that such a simple mathematical model of metal solidification rendered a very good approximation of the experimental data.

## Acknowledgements

I would like to express my gratitude to Mirosława Pawlyta, Waldemar Kwaśny and Mariusz Król for their assistance in obtaining the experimental data.

This research was financed by the resources allocated in years 2007-2009 under research project N N512 3348 33.

The calculations were made at the Warsaw University Interdisciplinary Centre for Mathematical and Computational Modelling (ICM) under computational grant no. G30-7.

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