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Calculation of the cooling condition in the phase change problem

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Analysis and modelling

ABSTRACT

Purpose: The purpose of the paper is to present the method of calculation of the cooling condition in the phase change problem. The considered problem consists of the reconstruction of a function describing the heat transfer coefficient, when the temperature values in selected points of the solid phase are known.
Design/methodology/approach: In numerical calculations, the Tikhonov regularization, the genetic algorithm and the alternating phase truncation method were used.
Findings: The featured examples of calculations show a very good approximation of the exact solution and stability of the procedure.
Practical implications: The paper presents an example of selection of the heat transfer coefficient given in the form of a continuous function. This method can be easily adopted also for the determination of other parameters of the problem discussed here.
Originality/value: The calculations made, only part of which has been presented in this paper, show stability of the method proposed, both in terms of the input data errors and the number of control points, thus corroborating usefulness of the presented approach.
Keywords: Solidification; Inverse Stefan Problems; Genetic algorithm; Tikhonov Regularization

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1. Introduction

The mathematical models of a number of significant phenomena to be found in practice lead to different types of ill-conditioned inverse problems for mathematical physics equations and, in particular, to incorrectly posed problems for the heat conduction equation. In general, such problems appear while trying to reconstruct the course of a process described by a correctly posed problem based on the results of measurements which should unequivocally determine the solution, but they do not do so in a correct way. Inverse problems for mathematical physics equations consists of the determination of e.g. the initial condition, the boundary conditions or the parameters of the material. The missing part of input information is compensated for with additional information, whose consequences result from the input conditions.

A two-phase Stefan problem is a mathematical model of solidification of pure metals. It consists of determining the temperature distributions in a solid and a liquid phase, and defining the positions of moving interfaces (freezing front) when the initial condition, boundary conditions and the thermophysical properties of a body are known. In the inverse Stefan problem, the lack of information about part of initial conditions is compensated for with information about the knowledge of the moving interface position, its speed of shifting in a normal direction or the temperature in selected points of the domain.

It is possible to find an exact analytical solution of the inverse Stefan problem only in a few simple cases. In other cases we are left with approximate solutions only. Grzymkowski and Słota (2006) [1] used the Adomian decomposition method combined with optimization for an approximate solution of a one-phase inverse Stefan problem. However, Słota [2] applies the variational iteration method to the discussed problems. To solve an inverse design Stefan problem, where a function describing the boundary condition is to be determined, Ren [3] takes advantage of the heat balance integral method. The author assumes that the temperature distribution in a solid phase is described by means of a third degree polynomial. Zabaras [4,5] considers a case where the additional information is the knowledge of temperature in selected points of the solid phase, and the interface position and its speed [4], or the heat flux on the domain boundary [5], are to be found. Liu [6] compares selected numerical methods to solve a one-dimensional, one-phase inverse Stefan problem.

An inverse Stefan problem was also applied in the modeling of the evaporation process [7], diffusion [8] or ablation [9,10]. In the works of Budman *et al.* [11], Rabin and Shitzer [12], an inverse Stefan problem was applied for the study and description of the solidification process taking place in biological tissues.

There are also other papers available, which deal with various problems connected with solidification or heat treatment of different materials [13-19].

This paper presents an algorithm which enables solving a two-phase inverse Stefan problem, where the heat transfer coefficient was determined for one of the domain boundaries. Based on the given information about the values of temperature in selected points of the solid phase, a functional determining the error of an approximate solution was built. To find the minimum of the functional, a genetic algorithm was applied [20,21] and to solve the direct Stefan problem, the alternating phase truncation method was used [22,23]. The inverse Stefan problem belongs to ill-conditioned problems, meaning that its solution is unstable due to the errors of input data. This means that insignificant errors at the input may cause significant errors at the output. For the avoidance of such behavior, appropriate stabilizing procedures are applied. Here, the Tikhonov regularization method is used owing to the accuracy and stability of the results obtained [24,25]. In Słota's papers [26,27], an analogical method was applied to solve an inverse design Stefan problem.

2. Two-phase problem

We will consider a two-phase problem. The boundary of the considered domain $D=[0,b]\times[0,t^*]$ will be divided into five parts (Fig. 1):

$$\Gamma_0=\{(x,0),x\in[0,b]\},$$
$$\Gamma_{11}=\{(0,t),t\in[0,t_k]\},\qquad \Gamma_{12}=\{(0,t),t\in[t_k,t^*]\},$$
$$\Gamma_{21}=\{(b,t),t\in[0,t_p]\},\qquad \Gamma_{22}=\{(b,t),t\in[t_p,t^*]\},$$

for which an initial condition and boundary conditions are predefined. 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 will be denoted as Γ_g. Let us assume that it is described by function $x=\xi(t)$. We will look for an approximate solution of the following problem.

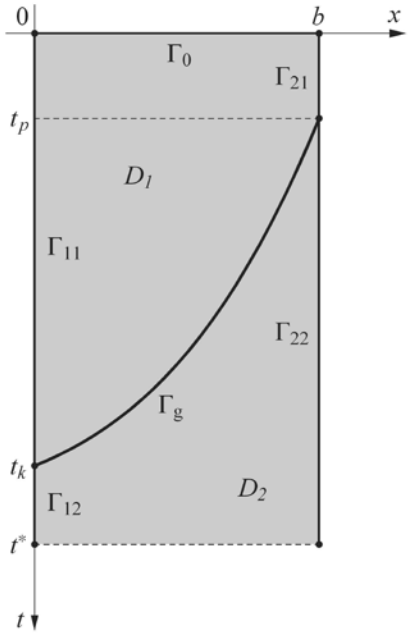


Fig. 1. Domain of the two-phase problem

With the known values of temperatures in selected points of the solid phase ($(x_i,t_j)\in D_2$):

$$T_2(x_i,t_j)=U_{ij},\qquad i=1,2,\ldots,N_1,\quad j=1,2,\ldots,N_2, \tag{1}$$

where N_1 means the number of sensors and N_2 means the number of measurements from each sensor, function $\alpha(t)$ defined on boundaries Γ_{2k} ($k=1,2$) is to be determined, and function $\xi(t)$ describing the moving interface position and the distribution of temperatures T_k in domains D_k ($k=1,2$), which inside domains D_k ($k=1,2$) fulfil the heat conduction equation:

$$c_k\rho_k\frac{\partial T_k}{\partial t}(x,t)=\lambda_k\frac{\partial^2 T_k}{\partial x^2}(x,t), \tag{2}$$

on boundary Γ_0, they fulfil the initial condition

$$T_1(x,0)=T_0, \tag{3}$$

on boundaries Γ_{1k} ($k=1,2$), they fulfil the homogeneous second kind conditions:

$$\frac{\partial T_k}{\partial x}(0,t)=0, \tag{4}$$

on boundaries Γ_{2k} ($k=1,2$), they fulfil the third kind conditions:

$$-\lambda_k \frac{\partial T_k}{\partial x}(b,t)=\alpha(t)\left(T_k(b,t)-T_\infty\right), \tag{5}$$

whereas on the moving interface Γ_g, they fulfil the temperature continuity condition and the Stefan condition:

$$T_1(\xi(t),t)=T_2(\xi(t),t)=T^*, \tag{6}$$

$$-\lambda_1 \frac{\partial T_1(x,t)}{\partial x}\bigg|_{x=\xi(t)}+\lambda_2 \frac{\partial T_2(x,t)}{\partial x}\bigg|_{x=\xi(t)}=L\rho_2 \frac{d\xi(t)}{dt}, \tag{7}$$

where c_k, ρ_k and λ_k are the specific heat, the mass density and the thermal conductivity in the liquid phase ($k=1$) and solid phase ($k=2$), respectively, α is the heat transfer coefficient, T_0 is the initial temperature, T_∞ is the ambient temperature, T^* is the temperature of solidification, L is the latent heat of fusion, and t and x refer to time and spatial location, respectively.

The direct Stefan problem occurring from equations (2)-(7) for a given heat transfer coefficient was solved via the alternating phase truncation method. As a result, the temperature distribution in the solid phase was obtained, constituting the reference point for a comparison of results. From the distribution, temperatures U_{ij}, simulating the temperature measurements, are obtained. Further in the paper, the so obtained temperatures will be treated as accurate.

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:

$$\alpha(t)=\alpha(t;\alpha_1,\alpha_2,\ldots,\alpha_n). \tag{8}$$

Let V denotes a set of all functions in the form of (8). 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:

$$V_\alpha=\left\{\alpha(t)\in V,\alpha_i\in\left[\alpha_i^l,\alpha_i^u\right]\right\}. \tag{9}$$

For the determined function $\alpha(t)\in V_\alpha$, the problem (2)-(7) becomes a direct Stefan problem, the solution of which allows finding the courses of temperatures $T_{ij}=T_2(x_i,t_j)$ corresponding to function $\alpha(t)$. By taking advantage of the calculated temperatures T_{ij} and the given temperatures U_{ij}, we can build a functional which will determine the error of the approximate solution:

$$J(\alpha(t))=\|T-U\|^2+\gamma\|\alpha(t)\|^2, \tag{10}$$

where γ is the regularization parameter and

$$\|T-U\|^2=\sum_{i=1}^{N_1}\sum_{j=1}^{N_2}\left(T_{ij}-U_{ij}\right)^2, \tag{11}$$

$$\|\alpha(t)\|^2=\int_0^{t^*}\omega(t)(\alpha(t))^2\,dt, \tag{12}$$

$\omega(t)$ is a weight function.

To determine the regularization parameter, the discrepancy principle proposed by Morozov was used, according to which the regularization parameter is determined from the equality:

$$\|T-U\|^2=\delta, \tag{13}$$

where δ is error estimation of the input data U. In practice, for a selected set of values γ_j, $j=0,1,\ldots,n$ of the regularization parameter, there is element T_{γ_j} minimizing the Tikhonov functional (10). Next, such value γ_{j_0} is selected as the sought regularization parameter, for which equation (13) is satisfied with the required accuracy.

3. Genetic algorithm

To find the Tikhonov functional minimum, a genetic algorithm was used. For the representation of the vector of decision variables, a chromosome was used in the form of a vector of real numbers (real number representation). The tournament selection was applied in the algorithm. This selection is carried out so that two chromosomes are drawn and the one with better fitness, goes to a new generation. There are as many draws as individuals that the new generation is supposed to include.

As the crossover operator, arithmetical crossover was applied, where as a result of crossing of two chromosomes α^1 and α^2, their linear combinations are obtained:

$$\begin{aligned}\overline{\alpha}^1&=r\alpha^1+(1-r)\alpha^2,\\ \overline{\alpha}^2&=r\alpha^2+(1-r)\alpha^1,\end{aligned} \tag{14}$$

where parameter r 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 α_i gene is transformed according to the equation:

$$\overline{\alpha}_i=\begin{cases}\alpha_i+\Delta(\tau,\alpha_i^u-\alpha_i),\\ \alpha_i-\Delta(\tau,\alpha_i-\alpha_i^l),\end{cases} \tag{15}$$

and a decision is taken at random which from the above formulas should be applied, where:

$$\Delta(\tau, x) = x\left(1 - r^{(1-\tau/N)d}\right), \tag{16}$$

and r is a random number with a uniform distribution from the domain $[0,1]$, τ is the current generation number, N is the maximum number of generations and d is a constant parameter.

The elitist model was applied in the algorithm. In this model 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 saved best individual from the previous population. The parameters of the genetic algorithm used in calculations are presented in Table 1.

Table 1.
Parameters of the genetic algorithm

Population size	70
Number of generations	500
Crossover probability	0.7
Mutation probability	0.1
Parameter of nonuniform mutation	2.0

4. Calculation example

Now we will present an example illustrating the accuracy and stability of the presented algorithm. In the presented example, the following values were assumed for the parameters: $b = 0.08$ [m], $\lambda_1 = 33$ [W/(m K)], $\lambda_2 = 30$ [W/(m K)], $c_1 = 800$ [J/(kg K)], $c_2 = 690$ [J/(kg K)], $\rho_1 = 7000$ [kg/m^3], $\rho_2 = 7500$ [kg/m^3], $L = 270000$ [J/kg], $T^* = 1773$ [K], $T_\infty = 323$ [K] and $T_0 = 1813$ [K].

In the alternating phase truncation method, the finite difference method was utilized, and the calculations were carried out on a grid with discretization steps equal $\Delta t = 0.1$ and $\Delta x = b/500$. A (reasonable) change of the grid density did not have any significant influence on the results obtained.

Function $\alpha(t) = \alpha(t; \alpha_1, \alpha_2, \alpha_3, \alpha_4)$ was sought in the form (Fig. 2):

$$\alpha(t) = \begin{cases} \dfrac{\alpha_2 - \alpha_1}{t_1} t + \alpha_1 & for \quad t \in [0, t_1], \\ \dfrac{\alpha_3 - \alpha_2}{t_2 - t_1} t + \dfrac{\alpha_3 t_2 - \alpha_2 t_1}{t_2 - t_1} & for \quad t \in (t_1, t_2], \\ \alpha_3 \exp\left(\dfrac{\ln(\alpha_4/\alpha_3)}{t_3 - t_2}(t - t_2)\right) & for \quad t \in (t_2, t^*], \\ \alpha_3 \exp\left(\dfrac{\ln(\alpha_4/\alpha_3)}{t_3 - t_2}(t^* - t_2)\right) & for \quad t > t^*, \end{cases}$$

where $t_1 = 38$ [s], $t_2 = 93$ [s], $t_3 = 350$ [s], $t^* = 750$ [s]. The set of constraints V_α was determined in the following way:

$$V_\alpha = \{\alpha(t); \alpha_1 \in [1100, 1500], \alpha_2 \in [600, 900], \alpha_3 \in [500, 800], \alpha_4 = [200, 400]\}$$

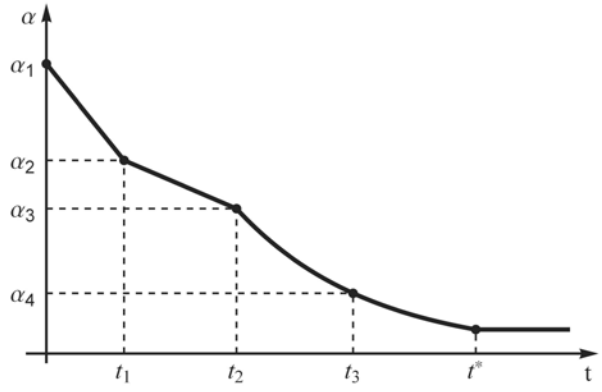


Fig. 2. Function $\alpha(t)$

The exact values of the sought coefficients α_i were:
$\alpha_1 = 1200$, $\alpha_2 = 800$, $\alpha_3 = 600$, $\alpha_4 = 250$.

It was assumed that in the domain under consideration three thermocouples were present ($N_1 = 3$), located at a distance of 5 [mm] (position A), 10 [mm] (position B) and 15 [mm] (position C) from the domain boundary (Fig. 3). The temperature was read out every 1 [s], 2 [s], 4 [s] or 8 [s]. This corresponded to a situation where from each thermocouple, 100, 50, 25 or 12 measured temperature values were obtained, respectively.

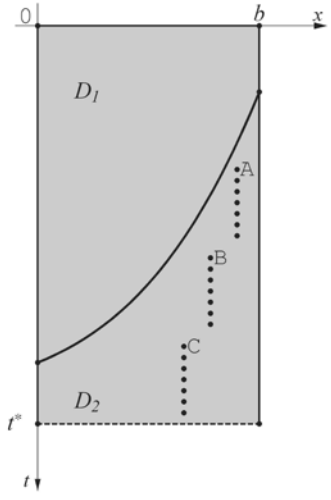


Fig. 3. Positions of the measurement points

Tables 2-5 present the results of calculations of the sought heat transfer coefficient values (averages from ten runs of the genetic algorithm). The tables also show the relative percentage errors, with which the values were determined, the standard

deviations obtained for ten runs of the genetic algorithm and the values of such standard deviations, expressed as percent of mean value. For the input data given without perturbations, the heat transfer coefficient values are very well reconstructed (errors do not exceed 0.009%). As perturbation grows, the errors of the heat transfer coefficient reconstruction increase, however, they do not exceed the input data errors in any case.

As can be seen from the presented results, the differences in solutions obtained for different numbers of control points are insignificant.

Table 2.
Calculation results for temperature control performed every second (α - reconstructed values of the heat transfer coefficient, e - relative percentage error, σ - standard deviation, σ^p - standard deviations in percent of mean value)

Per.	α	e [%]	σ	σ^p [%]
0%	1199.95	0.003964	0.109113	0.009093
	800.04	0.004469	0.057014	0.007126
	599.99	0.001708	0.032180	0.005363
	249.99	0.000850	0.016251	0.006500
1%	1204.07	0.339382	0.095254	0.007911
	795.09	0.613802	0.053767	0.006762
	602.28	0.379708	0.033769	0.005607
	248.86	0.456167	0.021313	0.008564
2%	1187.60	1.033462	0.117396	0.009885
	806.33	0.791670	0.064906	0.008050
	598.19	0.301788	0.029093	0.004863
	250.69	0.274182	0.012773	0.005095

Table 3.
Calculation results for temperature control performed every two seconds (designations identical to those in Table 2)

Per.	α	e [%]	σ	σ^p [%]
0%	1199.89	0.008948	0.148247	0.012355
	800.06	0.007570	0.086612	0.010826
	599.99	0.002271	0.039972	0.006662
	250.01	0.002275	0.023323	0.009329
1%	1202.45	0.204299	0.069795	0.005804
	798.12	0.234813	0.035535	0.004452
	598.77	0.205319	0.017628	0.002944
	251.31	0.525000	0.009596	0.003818
2%	1188.22	0.981556	0.060388	0.005082
	802.73	0.341854	0.036286	0.004520
	603.52	0.586500	0.028089	0.004654
	248.67	0.531700	0.017147	0.006895

Table 4.
Calculation results for temperature control performed every four seconds (designations identical to those in Table 2)

Per.	α	e [%]	σ	σ^p [%]
0%	1199.92	0.006833	0.141807	0.011818
	800.06	0.007841	0.094688	0.011835
	599.99	0.002379	0.028945	0.004824
	249.99	0.000473	0.014237	0.005695
1%	1189.01	0.915549	0.090959	0.007650
	802.44	0.305104	0.043472	0.005417
	600.95	0.157611	0.026862	0.004470
	250.56	0.225667	0.012844	0.005126
2%	1209.16	0.763500	0.097776	0.008086
	794.69	0.664075	0.076037	0.009568
	596.40	0.600417	0.039720	0.006660
	253.41	1.365920	0.019161	0.007561

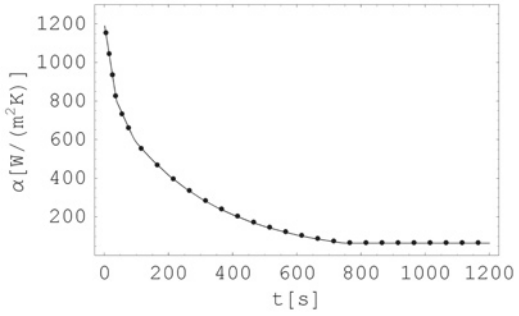
Table 5.
Calculation results for temperature control performed every eight seconds (designations identical to those in Table 2)

Per.	α	e [%]	σ	σ^p [%]
0%	1199.9	0.008788	0.104008	0.008668
	800.0	0.008341	0.063568	0.007945
	599.9	0.003894	0.028298	0.004717
	250.0	0.003564	0.011341	0.004536
1%	1190.08	0.826764	0.138199	0.011613
	802.71	0.339031	0.072219	0.008997
	601.06	0.176847	0.045261	0.007530
	248.69	0.525933	0.024745	0.009950
2%	1193.21	0.566192	0.055793	0.004676
	792.70	0.912400	0.037100	0.004680
	601.67	0.278767	0.024096	0.004005
	249.55	0.181240	0.014103	0.005651

Figure 4 presents an accurate and reconstructed course of the heat transfer coefficient $\alpha(t)$ variability for temperature control every four seconds and every eight seconds, and perturbation of 2%. The relative percentage error of the reconstruction of function $\alpha(t)$ amounted to 0.202% and 0.008%, respectively. In other cases, the function describing the heat transfer coefficient was determined with equally insignificant errors.

Figure 5 presents accurate and reconstructed temperature distributions in control points (A, B and C), also for temperature control performed every four seconds and every eight seconds, and perturbation of 2%. Where temperature control was performed every four seconds, the mean relative percent error was 0.33%, with the maximum relative percent error amounting to 0.74%. This was the worst result obtained during the calculations, however, the errors with which the temperature distributions were reconstructed are significantly lower than the input data error. In the latter result presented here, the errors were 0.09% and 0.19%, respectively. In the remaining cases, results with similarly small errors were obtained.

a)



b)

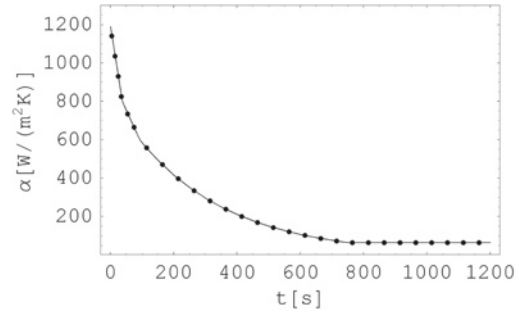
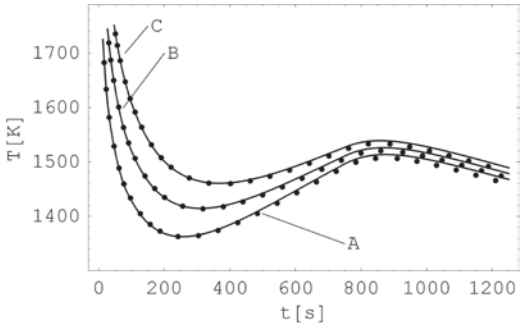


Fig. 4. Exact (solid line) and reconstructed (dots) distribution of the heat transfer coefficient for perturbation equal to 2%, and for temperature control every four seconds (a) and every eight seconds (b)

a)



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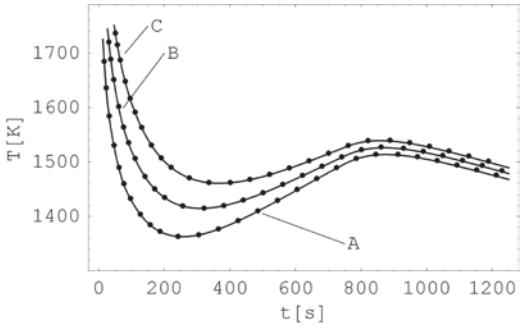
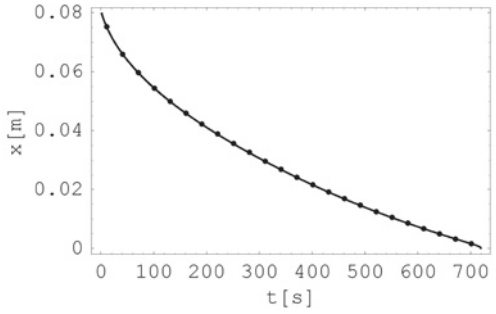


Fig. 5. Exact (solid line) and reconstructed (dots) distributions of the temperature in the measurement points for perturbation equal to 2%, and for temperature control every four seconds (a) and every eight seconds (b)

a)



b)

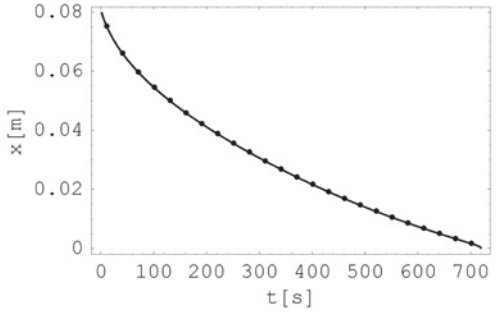


Fig. 6. Exact (solid line) and reconstructed (dots) position of the freezing front for perturbation equal to 2%, and for temperature control every four seconds (a) and every eight seconds (b)

Figure 6 presents an accurate and reconstructed position of the freezing front obtained for temperature control performed every four seconds and every eight seconds, and perturbation of 2%. The mean relative percent errors, with which the freezing front position was reconstructed, were similar and amounted to 0.75% and 0.76%, respectively. For a larger number of control points, the errors were lower and amounted to 0.31% for temperature control conducted every two seconds and 0.11% for temperature control performed every second (with the same perturbation of 2%).

5. Conclusions

The paper presents the determination method of cooling conditions in the phase change process. The solution of the problem consisted of selecting a heat transfer coefficient on one boundary, so that the temperature in selected points of the solid phase would assumed the given values. In the elaborated algorithm, the alternating phase truncation method, the Tikhonov regularization and genetic algorithms were utilized.

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, however, that the sought boundary condition should be linearly dependent on those parameters. Since

anon-gradient optimization method was applied for the minimization of the functional so built, the minimized functional may also non-linearly depend on the parameters sought.

The results presented in the paper show that for the input data given without perturbation, the function describing the cooling conditions is reconstructed with minimal errors being the consequence of the assumed end of the numerical procedure. A reduction of the number of control points, with accurate input data, does not cause any significant changes in the reconstructed boundary condition. The calculations made, only part of which has been presented in this paper, show stability of the method proposed, both in terms of the input data errors and the number of control points, thus corroborating usefulness of the presented approach.

The paper presents an example of selection of the heat transfer coefficient given in the form of a continuous function. This method can be easily adopted also for the determination of other parameters of the problem discussed here.

Acknowledgements

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