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NUMERICAL METHOD FOR MULTI-PHASE INVERSE STEFAN DESIGN PROBLEMS

METODA NUMERYCZNA ROZWIĄZANIA WIELOFAZOWEGO ODWROTNEGO PROJEKTOWEGO ZAGADNIENIA STEFANA

The inverse problems for differential equations consist of stating the initial conditions, boundary conditions or thermophysical properties of the body. But the insufficiency of input information is compensated by some additional information on the effects of the input conditions. Generally, for the inverse Stefan problem, it is assumed that this additional information is the position of the freezing front, its velocity in normal direction or temperature in selected points of the domain. We may consider the usage of the demanded position of the moving front as the constraint for the cost functional. This kind of problem becomes an inverse design problem.

In the paper, the multi-phase inverse Stefan design problems are formulated and described by means of the optimization method. These problems consist of the reconstruction of the function which describes the heat-transfer coefficient, when the positions of the moving interfaces of the phase change are well-known. The method consists of the minimization of a functional, the value of which is the norm of a difference between given position of the moving interface of the phase change and a position reconstructed from the selected function describing the heat-transfer coefficient. In numerical calculations the Nelder-Mead optimization method and the generalized alternating phase truncation method were used.

Keywords: Inverse Stefan Design Problems, Solidification, Generalized Alternating Phase Truncation Method, Nelder-Mead Method.

Modele matematyczne szeregu istotnych zjawisk spotykanych w praktyce prowadzą do różnych typów źle uwarunkowanych zagadnień odwrotnych dla równań fizyki matematycznej, a w szczególności do niepoprawnie postawionych zagadnień dla równania przewodnictwa ciepła. Na ogół zagadnienia te pojawiają się przy próbach odtworzenia przebiegu jakiegoś procesu opisanego zagadnieniem poprawnie postawionym, na podstawie wyników pomiarów, które powinny jednoznacznie określić rozwiązanie, ale nie czynią tego w sposób poprawny. Zagadnienia odwrotne dla równań fizyki matematycznej polegają na określeniu np. warunku początkowego, warunków brzegowych lub parametrów materiału. Brak pewnej części informacji wejściowej, jest uzupełniany dodatkowymi informacjami o konsekwencjach wynikłych z warunków wejściowych. Dla odwrotnego zagadnienia Stefana dodatkową informacją jest znajomość położenia granicy rozdziału faz, jej prędkości w kierunku normalnym lub temperatury w wybranych punktach obszaru. W przypadku, gdy do budowy funkcji celu wykorzystamy żądane położenie granicy rozdziału faz, to tego typu zadanie nosi nazwę odwrotnego zagadnienia projektowego.

W pracy będziemy rozważać wielofazowe odwrotne projektowe zagadnienie Stefana, w których dodatkową informacją są położenia granic rozdziału faz. W opisywanej metodzie dobierana będzie wartość (zmiennego w czasie) współczynnika wnikania ciepła, tak aby zminimalizować funkcjonał, którego wartością jest norma różnicy między zadanym położeniem granicy rozdziału faz i położeniem odtworzonym dla wybranego współczynnika wnikania ciepła. W obliczeniach numerycznych wykorzystano metodę optymalizacji Neldera-Meada oraz uogólnioną metodę przemiennej fazy.

1. Introduction

The inverse problems for differential equations consist of stating the initial conditions, boundary conditions or thermophysical properties of the body. But the insufficiency of input information is compensated by some additional information on the effects of the input conditions. Generally, for the inverse Stefan problem, it is assumed that this additional information is the position of the freezing front, its velocity in normal direction or temperature in selected points of the domain. We may consider the usage of the demanded position of the moving front as the constraint for the cost functional. This kind of problem becomes an inverse design problem.

Most of the papers concerning this field are focused on the one-phase one-dimensional inverse Stefan problems. Papers devoted to two-dimensional problems are not that numerous, part of them have little importance

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for applications, as regards a way of solution [1, 2, 5, 7, 22]. Most published materials involve the reconstruction of temperature or heat flux on the boundary of a domain [2, 3, 28-31]. In paper [27] the distribution of the inner heat sources in a domain is reconstructed. The inverse Stefan problems, where the thermal properties of materials (e.g. thermal conductivity, thermal diffusivity, coefficient of convective heat-transfer etc.) are reconstructed, are discussed in papers [22-25]. Unfortunately, all these papers pertain to semiinfinite domains, but the two-phase problem is considered only in paper [22].

In papers [1, 2, 10, 26] the regularization of inverse Stefan problems and the system of linear Volterra integral equations obtained is turned into a linear Volterra equation of the second kind associated with an equation of the convolution type. In paper [7] the solution is found in terms of an infinite series of one-dimensional integrals. Jochum [16] considers the inverse Stefan problem as a problem of nonlinear approximation theory (see [14, 15]). In papers [8, 9] for solutions of one-phase two-dimensional problems the authors used a complete family of solutions of the heat equation to minimize the maximal defect in the initial-boundary data. Similar method was used for one- and two-dimensional two-phase inverse Stefan problems in [11-13]. In this method, the solution is found in a linear combination form of the functions satisfying the equation of heat conduction. The coefficients of this combination are determined by the least square method for the boundary of a domain. In papers [4, 17, 32, 33] the authors used dynamic programming or minimization techniques in finite- and infinite dimensional space. Unfortunately, the majority of these papers pertain to the one-phase problems, the two-phase problems are considered only in papers [2, 12, 13, 17, 32, 33].

In this paper, a mthod for the reconstruction of the function which describes the heat-transfer coefficient is discussed, when the position of the moving interface of the phase change is well-known. The method consists of the minimization of a functional, the value of which is the norm of a difference between given position of the moving interface of the phase change and a position reconstructed from the selected function describing the heat-transfer coefficient. In numerical calculations the Nelder-Mead optimization method [6, 20] and the generalized alternating phase truncation method [18, 21] were used.

2. Formulation of the problem

Let $\Omega = (a, b) \subset \mathbb{R}$. On the boundary of a domain $D = \Omega \times (0, t^*)$ three components are distributed:

$$\Gamma_0 = \{(x, 0); x \in [a, b]\}, \tag{1}$$

$$\Gamma_1 = \{(a, t); t \in [0, t^*]\}, \tag{2}$$

$$\Gamma_2 = \{(b, t); t \in [0, t^*]\}, \tag{3}$$

where initial and boundary conditions are given. Let D_k $(k = 1, \ldots, n)$ be this subset of domain D which is occupied by k phase. Domains D_k and D_{k+1} are separated by the moving interface $\Gamma_{k,k+1}$ $(x = \xi_{k,k+1}(t))$, $k = 1, \ldots, n-1$. We will look for an approximate solution of the following problem:

For given positions of moving interfaces $\Gamma_{k,k+1}$, the distribution of temperature T_k in domain D_k $(k = 1, \ldots, n)$ is calculated, as well as function $\alpha(t)$ on boundary Γ_2, which satisfies the following equations (for $k = 1, \ldots, n$):

$$c_k \rho_k \frac{\partial T_k}{\partial t}(x, t) = x^{-l} \frac{\partial}{\partial x}\left(\lambda_k x^l \frac{\partial T_k}{\partial x}(x, t)\right), \quad \text{in } D_k, \tag{4}$$

$$T_1(x, 0) = \varphi_0(x), \quad \text{on } \Gamma_0, \tag{5}$$

$$-\lambda_k \frac{\partial T_k}{\partial x}(a, t) = 0, \quad \text{on } \Gamma_1, \tag{6}$$

$$-\lambda_k \frac{\partial T_k}{\partial x}(b, t) = \alpha(t)(T_k(b, t) - T_\infty), \quad \text{on } \Gamma_2, \tag{7}$$

$$T_k(x, t) = T^*_{k-1,k}, \quad \text{on } \Gamma_{k-1,k}, \tag{8}$$

$$T_k(x, t) = T^*_{k,k+1}, \quad \text{on } \Gamma_{k,k+1}, \tag{9}$$

$$L_{k,k+1}\rho_{k+1}\frac{d\xi_{k,k+1}(t)}{dt} = -\lambda_k \frac{\partial T_k(x, t)}{\partial x}\bigg|_{\Gamma_{k,k+1}} + \lambda_{k+1}\frac{\partial T_{k+1}(x, t)}{\partial x}\bigg|_{\Gamma_{k,k+1}}, \tag{10}$$

where $l = 0$ for one-dimensional problems and $l = 1$ for axisymmetrical problems, c_k are the specific heat in k phase, ρ_k are mass density, λ_k thermal conductivity, α heat-transfer coefficient, $T^*_{k,k+1}$ temperature of the phase change, T_∞ ambient temperature, $L_{k,k+1}$ latent heat of fusion between k and $k+1$ phase.

Let's assume that functions $\xi^*_{k,k+1}$ describing the exact position of the moving interfaces are well-known. Function α is designated in the form:

$$\alpha(t) = \begin{cases} \alpha_1 & \text{for } t \in [0, t_{\alpha_1}], \\ \alpha_2 & \text{for } t \in (t_{\alpha_1}, t_{\alpha_2}], \\ \vdots & \\ \alpha_{N-1} & \text{for } t \in (t_{\alpha_{N-2}}, t_{\alpha_{N-1}}], \\ \alpha_N & \text{for } t \in (t_{\alpha_{N-1}}, t^*). \end{cases} \quad (11)$$

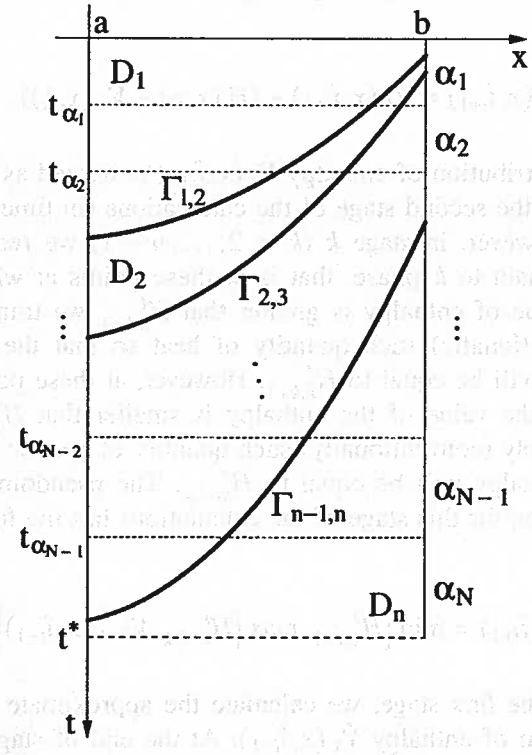

Fig. 1. Domain of the multi-phase problem

Let V_α denote the set of all functions in form (11), where $\alpha_i \in \mathbb{R}$. In real processes function $\alpha(t)$ describing the heat-transfer coefficient doesn't have an arbitrary value. Therefore, the problem of minimization with constraints has some practical application. Assuming that:

$$V_\alpha^0 = \{\alpha \in V_\alpha, \alpha_i \geqslant 0\}, \quad (12)$$

$$V_\alpha^p = \{\alpha \in V_\alpha, \alpha_i \in [p_{1i}, p_{2i}]\}, \quad (13)$$

For fixed function $\alpha \in V$, where $V = V_\alpha^0$ or $V = V_\alpha^p$, the problem in (4)-(10) the direct multi-phase Stefan problem occurs and its solution makes it possible to find the positions of the moving interfaces corresponding to function $\alpha(t)$.

Let's assume that functions $\xi_{k,k+1}^*$ for $k = 1, \ldots, n-1$ describing the exact positions of the moving interfaces are well-known. The minimized discrete functional can be represented as:

$$J(\alpha(t)) = \left(\sum_{k=1}^{n-1} \sum_{p=1}^{M} \left[w(t) \left(\xi_{k,k+1,p} - \xi_{k,k+1,p}^* \right)^2 \right] \right)^{1/2}, \quad (14)$$

where $w(t)$ is the weight function, equalizing the influence of the length of the zones and M is the number of points of the discretization of the moving interfaces.

The size of the gradient of temperature in the solid zone exerts a considerable influence on the properties of ready casts (big values of the gradient evoke the formation of cracks) [19]. Therefore, in the minimization procedure it is advisable to consider the second criterion, minimizing the gradient of temperatures in the solid zone. To achieve this, the following functionals are introduced [19]:

$$I_1(\alpha(t)) = \left(\int_{D_n} |\nabla T_n|^2 \, dxdt \right)^{1/2} \quad (15)$$

and

$$I(\alpha(t)) = \omega_1 J(\alpha(t)) + \omega_2 I_1(\alpha(t)), \quad (16)$$

where ω_i are weight coefficients. In the problem with constraints we will look for such element of $\alpha_m \in V$, where $V = V_\alpha^0$ or $V = V_\alpha^p$, that would fulfill the following condition:

$$I(\alpha_m) = \inf_{\alpha \in V} I(\alpha). \quad (17)$$

To look for the minimum of functional Iwe used the Nelder-Mead optimization method [6, 20]. However, for solving the direct multi-phase Stefan problem (4)-(10), for fixed function α, we used the generalized alternating phase truncation method [18, 21].

3. Generalized alternating phase truncation method

For solving direct Stefan problem the alternating phase truncation method may be used, which was worked out by Rogers, Berger and Ciment [21]. This method belongs to the fixed domain methods, which try to transform the problem or the way of solving so that the Stefan condition occurred in the open form. The method presented in paper [21] is applied to two-phase problems. Expanded application of this method in the case of multi-phase is presented in paper [18].

In the alternating phase truncation method in place of temperature which occurred in the Stefan problem we insert an enthalpy:

$$H(T) = \int_0^T c(u) \varrho(u) \, du + \sum_{k=1}^{n-1} \eta_{k,k+1}(T) L_{k,k+1} \varrho_{k+1}, \quad (18)$$

where

$$\eta_{k,k+1}(T) = \begin{cases} 1 & \text{for } T > T^*_{k,k+1}, \\ 0 & \text{for } T \leqslant T^*_{k,k+1}. \end{cases} \tag{19}$$

From this definition it follows that this is an increasing function. Thus, there is an inverse function:

$$T = \Theta(H), \tag{20}$$

enabling the calculation of temperature on the basis of enthalpy. Function $H(T)$ is discontinuous in the points given by the temperatures of the phase change $T^*_{k,k+1}$. Its left-hand and right-hand limits at these points will be denoted as: $H^l_{k,k+1}$ and $H^r_{k,k+1}$.
If we use the equation (18) in the Stefan problem, we will obtain:

$$c_k \varrho_k \frac{\partial H_k}{\partial t}(x,t) = x^{-l} \frac{\partial}{\partial x}\left(\lambda_k x^l \frac{\partial H_k}{\partial x}(x,t)\right), \tag{21}$$

$$G\left(H_k, \frac{\partial H_k}{\partial n}\right)\Big|_\Gamma = 0, \tag{22}$$

$$H_k(x,0) = H(\varphi_0(x)), \tag{23}$$

$$H^l_{k,k+1} = H^r_{k,k+1} + L_{k,k+1}\varrho_{k+1}, \tag{24}$$

$$L_{k,k+1}\varrho_{k+1}\frac{d\xi_{k,k+1}}{dt} = -\, a_k \frac{\partial H_k(x,t)}{\partial n}\Big|_{\Gamma_{k,k+1}} + a_{k+1}\frac{\partial H_{k+1}(x,t)}{\partial n}\Big|_{\Gamma_{k,k+1}}, \tag{25}$$

where the form of function G, describing the boundary conditions, depends on function $\Theta(H)$ and the boundary conditions. Function $H_k(T)$ narrows of function $H(T)$ down to the range of the temperature in k phase.

We assumed (for the simplicity of the description) that the phases are numbered from "the warmest" to "the coldest", i.e. D_1 denotes the domain of "the warmest" phase and D_n denotes the domain of "the coldest" phase. Let's assume that we know the distribution of enthalpy $H(x,t_i)$ in time t_i, from the initial condition or the previous step of the calculations. The algorithm of the generalized alternating phase truncation method (for one time's step) consists of n stages.

In the first stage we reduce all domain to "the warmest" phase, that is to these points at which the value of the enthalpy is smaller that $H^r_{1,2}$ we supply (conventionally) such quantity of heat so that enthalpy will be equal to $H^r_{1,2}$. The pseudoinitial condition for the first stage of the calculations has the form:

$$V_1(x,t_i) = \max\left\{H^r_{1,2}, H(x,t_i)\right\}.$$

The obtained one-phase heat conduction problem may be solved (for example) by the finite difference method or finite elements method. We get obtain the approximate distribution of enthalpy $\hat{V}_1(x,\hat{t}_{i+1})$. In these points at which we artificially supply some quantity of heat we must subtract this same quantity of heat, as follows:

$$V_1(x,\hat{t}_{i+1}) = \hat{V}_1(x,\hat{t}_{i+1}) + (H(x,t_i) - V_1(x,t_i)).$$

The distribution of enthalpy $V_1(x,\hat{t}_{i+1})$ is treated as initial for the second stage of the calculations (in time t_i).

However, in stage k ($k = 2,\ldots,n-1$) we reduce all domain to k phase, that is at these points at which the value of enthalpy is greater that $H^l_{k,k+1}$ we transfer (conventionally) such quantity of heat so that the enthalpy will be equal to $H^l_{k,k+1}$. However, at these points where the value of the enthalpy is smaller that $H^r_{k-1,k}$ we supply (conventionally) such quantity of heat so that the enthalpy will be equal to $H^r_{k-1,k}$. The pseudoinitial condition for this stage of the calculations has the form:

$$V_k(x,\hat{t}_{i+1}) = \min\left\{H^l_{k,k+1}, \max\left\{H^r_{k-1,k}, V_{k-1}(x,\hat{t}_{i+1})\right\}\right\}.$$

As in the first stage, we calculate the approximate distribution of enthalpy $\hat{V}_k(x,\hat{t}_{i+1})$. At the end of stage at these points where we artificially transferred (supplied) some quantity of heat we must add (subtract) this same quantity of heat:

$$V_k(x,\hat{t}_{i+1}) = \hat{V}_k(x,\hat{t}_{i+1}) + (V_{k-1}(x,\hat{t}_{i+1}) - V_k(x,\hat{t}_i)).$$

In the last stage ($k = n$) we reduce all domain to "the coldest" phase, that is to these points at which the value of the enthalpy is greater that $H^l_{n,n+1}$ we transfer (conventionally) such quantity of heat so that the enthalpy will be equal to $H^l_{n,n+1}$; and thus proceed as previously. The obtained distribution of enthalpy $H(x,t_{i+1}) = V_n(x,\hat{t}_{i+1})$ ends stage , as will as one step of the calculations (transfer from time t_i to t_{i+1}) for the generalized alternating phase truncation method.

In the generalized alternating phase truncation method for each time step the heat equation is solved many times (n). Therefore, we must take into consideration the boundary conditions, so that they influence on the system only by time Δt, and not by time $n \cdot \Delta t$ [18, 21].

4. Optimization

The Nelder-Mead method is a method of the minimization of the function of several variables. This method requires only function evaluations, not derivatives. The idea of the method consists in creating $(m+1)$-dimensional simplex. Then, the function values are compared at the simplex vertices. The simplex is transformed until the criterion of the ending procedure is fulfilled [6, 20].

In literature we can come across two kinds of the criterion the end of the procedure. In the first criterion [20], formulated by Nelder and Mead, the working of the iterative procedure is ended if the maximum of the distance between the points of the simplex and its center of gravity is smaller than some given number. Whereas, in the second criterion, formulated in [6], the working of the iterative procedure is ended if the standard deviation of the values of the function in the points of the simplex is smaller than some given number.

The criterion of the end of the procedure will be fulfilled if one of the inequalities (for $j = 1, 2$) is true:

$$\sigma_j < \varepsilon_j, \tag{26}$$

where, in the case of the first criterion:

$$\sigma_1 = \max_{i\in\{0,\ldots,m\}} |\alpha_s - \alpha_i| \tag{27}$$

or, in the case of the second criterion:

$$\sigma_2 = \sqrt{\sum_{i=0}^{m} \frac{\left(I_i - \bar{I}\right)^2}{m+1}}. \tag{28}$$

In the above equation I_i denotes the value of the minimized functional in point of the simplex, $\bar{I}$ denotes the mean value calculated on the basis of values of the minimized functional in the points of the simplex:

$$\bar{I} = \sum_{i=0}^{m} \frac{I_i}{m+1},$$

and α_s is barycentre:

$$\alpha_s = \frac{1}{m+1} \sum_{i=o}^{m} \alpha_i.$$

The values of the functional I we compute by solving the direct Stefan problem, derived from equations (4)–(10) for fixed heat-transfer coefficient and unknown positions of the moving interfaces $\Gamma_{k,k+1}$. As the ending criterion we assume the alternative of conditions (26) for $\varepsilon_1 = 1.0$ and $\varepsilon_2 = 10^{-7}$.

In Nelder-Mead method the simplex is transformed by four operations: reflection (with parameter $\bar{\alpha} > 0$), expansion (with parameter $\gamma > 1$), contraction (with parameter $\beta \in (0, 1)$) and reduction (multiple contraction) [6, 20]. Nelder and Mead suggest that the values of parameters $\bar{\alpha}$, γ and β should be taken as 1.0, 2.0 and 0.5, respectively.

The choice of the initial simplex was realized in such a way that point $\alpha_0 = \alpha_p$ was given; however, the other points were computed from the equation:

$$\alpha_i = \alpha_0 + ke_i, \quad i = 1, \ldots, m,$$

where e_i are the versors of the Cartesian coordinate system $\mathbb{R}^m$ and parameter k is equal to 300.

The programs calculating the algorithm of the presented method were written in *C++* and in language of the *Mathematica*.

5. Numerical examples

The theoretical considerations introduced in the previous sections will be illustrated with examples, in which we consider two- and three-phase problems for one-dimensional ($l = 0$) and axisymmetrical domain ($l = 1$).

The direct Stefan problem, derived from equations (4)–(10) for a fixed heat-transfer coefficient and unknown positions of the moving interfaces $\Gamma_{k,k+1}$, will be solved by the generalized alternating phase truncation method [18, 21]. Next, the found positions of the moving interfaces will be used as the input data for the inverse Stefan problem. In the next parts of this paper these positions will be called the exact positions of the moving interfaces.

The exact input data was perturbated by "measurement errors", generated by the generator of the pseudorandom numbers with uniform distribution. The calculations were done for some perturbation of the same and different values. The obtained results confirm the independence of the results from the random set of the perturbation.

5.1. Two-phase problems

In the examples we assumed the following values: $\Omega = (0, 0.08)$ [m], $\lambda_1 = 33$ [W/(m · K)], $\lambda_2 = 30$ [W/(m · K)], $c_1 = 800$ [J/(kg · K)], $c_2 = 800$ [J/(kg · K)], $\varrho_1 = 7000$ [kg/m^3], $\varrho_2 = 7500$ [kg/m^3], $L = 270000$ [J/kg], $T^*_{1,2} = 1773$ [K], $T_\infty = 323$ [K] and the initial temperature is equal to $\varphi_0(x) = 1813$ [K]. The exact value of the heat-transfer coefficient is equal to:

$$\alpha(t) = \begin{cases} 1200 & \text{for } t \in [0, t_{\alpha}], \\ 800 & \text{for } t \in (t_{\alpha_1}, t_{\alpha_2}], \\ 250 & \text{for } t \in (t_{\alpha_2}, t^*), \end{cases} \quad (29)$$

where $t_{\alpha_1} = 38$ [s], $t_{\alpha_2} = 93$ [s] and $t^* = 764$ [s].

Example 1

The first example concerns the solution of the one-dimensional two-phase inverse Stefan problem ($l = 0$). The minimum of functional (14) was designated in set V_{α}^{0}.

TABLE 1

Absolute values of percentage relative errors in the calculations for different starting points (calculations without weight coefficients, α_p – starting point, 1, 2, 3 – number of the zone)

Per.	α_p = (800, 800, 800)			α_p = (900, 900, 600)		
	1	2	3	1	2	3
0.0%	0.00	0.13	0.00	0.00	0.13	0.00
5.0%	1.75	1.00	0.80	1.58	0.88	0.40
10.0%	7.75	7.88	1.60	5.67	9.50	2.40
15.0%	9.83	6.50	0.40	11.92	9.25	0.80
20.0%	8.42	14.88	1.60	15.42	27.38	3.20
Per.	α_p = (850, 650, 350)			α_p = (1000, 700, 200)		
	1	2	3	1	2	3
0.0%	0.00	0.13	0.00	0.50	0.50	0.00
5.0%	2.08	0.50	0.80	2.08	1.50	0.40
10.0%	8.75	8.88	2.00	4.75	9.88	2.00
15.0%	2.25	2.50	2.40	1.75	1.88	1.20
20.0%	22.33	38.75	5.60	1.00	4.38	1.20

TABLE 2

Absolute values of percentage relative errors in the calculations for different starting points (calculations with weight coefficients, α_p – starting point, 1, 2, 3 – number of the zone)

Per.	α_p = (800, 800, 800)			α_p = (900, 900, 600)		
	1	2	3	1	2	3
0.0%	0.00	0.13	0.00	0.00	0.13	0.00
5.0%	0.08	3.25	1.60	0.58	3.00	1.20
10.0%	4.17	9.25	2.80	8.42	8.25	0.40
15.0%	3.92	5.38	2.40	0.42	2.00	1.60
20.0%	1.08	1.63	2.40	5.42	6.38	2.40
Per.	α_p = (850, 650, 350)			α_p = (1000, 700, 200)		
	1	2	3	1	2	3
0.0%	0.00	0.13	0.00	0.17	0.38	0.00
5.0%	3.75	3.38	0.00	1.75	1.00	2.00
10.0%	4.67	0.13	2.40	6.50	3.63	1.20
15.0%	2.75	2.25	2.80	0.58	4.13	2.40
20.0%	6.00	9.00	2.40	0.08	0.88	2.40

Tables 1 and 2 present the absolute values of percentage relative error in the reconstruction of the heat-transfer coefficient for different starting points and various sizes of the random noise in input data (in position of the moving interface). The results included in Table 1 have obtained when the weight coefficients are equals to one. This situation is equivalent to a situation where the weight coefficients were not included in the

functional (14). Therefore in the next parts of this paper this situation we will be called the situation without weight coefficients. However, the results included in Table 2 have been obtained when the weight coefficients are depending on the lengths of the zones (the coefficient increases with a decrease in the length of the zone). The sum of all coefficients is equal to one.

The obtained results show that for the input data without noise function is reconstructed with the accuracy to the errors arising out of the assumed moment of the end of the optimization process. The errors increase together with an increase in the noise in the input data. The heat-transfer coefficient is reconstructed very well for the noise not bigger than 15%. The errors in the reconstruction of the heat-transfer coefficient are significantly smaller than the errors in input data. However, if the noise equals to 20% for some of the starting points (α_p = (900,900,600)) and (α_p = (850,650,350)) the errors in the results, for the calculations without weight coefficient, are bigger than the errors in the input data. In this case, it turned out that the introduction of the weight coefficients has significantly improved the obtained results. However, for smaller noise, the introduction of the weight coefficients has not improved the obtained results significantly.

Out of all parameters describing the function α is the last parameter (α_3) is reconstructed best. This is connected with the length of the interval on which this parameter is given (α_1 is given on the interval (0,38], α_2 on the interval (38,93]; however, α_3 on the interval (93,764]), and even distribution of the control points, describing the position of the moving interface, most of the control points fall into the longer interval. The consideration of the weight coefficients in the calculations, in general insignificantly worsens the reconstruction of this parameter. However, it improves (in general) the reconstruction of the first and the second parameter of function α.

Figure 2 presents the results of the reconstruction of the moving interface, for the found function α_m (for starting point α_p = (800,800,800)). The exact position (solid line) and reconstructed position (dot line) of the moving interface are show in this figure. It follows from the calculations that irrespective of the given size of the noise in input data and the starting point the moving interface is reconstructed very well.

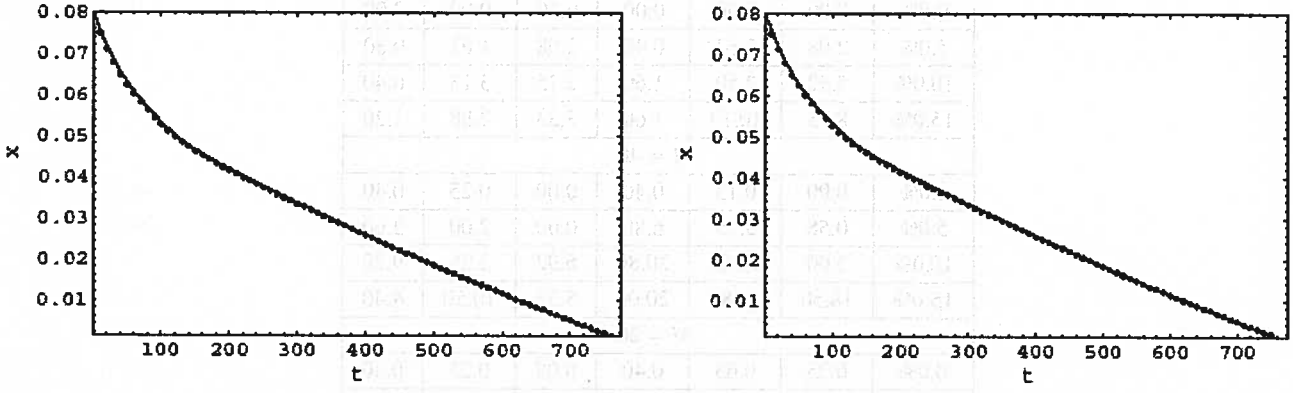

Fig. 2. Position of the freezing front reconstructed for the starting point α_p = (800, 800, 800) and data with perturbation equal to 5% (left figure), 15% (right figure) (solid line – exact position, dot line – reconstructed value)

Example 2

Now we will present the solution of the axisymetrical two-phase inverse Stefan problem (l = 1). The minimum of functional (14) was designated in sets V_α^0 and V_α^p for different number of the control points (ξ_j^*). Set V_α^p is defined as follows:

$$V_\alpha^p = \{\alpha \in V_\alpha; \alpha_1 \in [1000, 1500] \wedge \alpha_2 \in [500, 1000] \wedge \alpha_3 \in [150, 500]\}.$$

Table 3 presents the results obtained for the minimization in set V_α^0 for different starting points (α_p) and for forty control points (M = 40) describing the position of the moving interface. The obtained results confirm that the choice of the starting point does not have essential influence on the results of the reconstruction of function α. Even for a distant starting point such as point α_p = (0,0,0), at which the Robin condition is given on boundary Γ_2, it is transformed to Neumann condition with heat flux equal to zero, function α is reconstructed with the accuracy to the errors arising out of the assumed moment of the end of the optimization.

TABLE 3

Results of the calculations for different starting points (α_p – starting point, α_m – the found point of the minimum)

α_p			α_m		
α_{p1}	α_{p2}	α_{p3}	α_{m1}	α_{m2}	α_{m3}
1000	500	500	1200	800	250
1000	700	200	1200	802	249
900	900	600	1200	801	250
800	800	800	1198	801	250
700	300	450	1200	802	248
0	0	0	1201	799	251

Table 4 present the absolute values of the percentage relative errors in the reconstruction of the heat-transfer coefficient for the minimization of the functional in sets V_α^0 and V_α^p for giving (with and without noise) 398, 40 or 20 control points describing the position of the moving interface. Starting point α_p = (1000,500,500) was used in the calculations.

TABLE 4

Absolute values of the percentage relative errors in the calculations for different number of control points

Per.	V_α^0			V_α^p		
	1	2	3	1	2	3
M = 398						
0.0%	0.00	0.00	0.00	0.00	0.00	0.00
5.0%	2.08	2.63	0.40	2.08	1.63	0.80
10.0%	5.92	7.50	1.60	2.75	3.13	0.40
15.0%	8.75	10.13	1.60	3.33	2.88	1.20
M = 40						
0.0%	0.00	0.13	0.40	0.00	0.25	0.40
5.0%	0.58	5.75	6.80	0.00	2.00	3.60
10.0%	3.00	18.63	20.80	6.92	2.25	9.20
15.0%	18.50	33.88	20.00	5.33	10.50	4.40
M = 20						
0.0%	0.25	0.63	0.40	0.08	0.25	0.40
5.0%	7.50	7.50	0.80	1.25	6.63	2.00
10.0%	15.75	20.38	6.80	5.75	8.38	3.20
15.0%	13.17	25.88	14.80	3.42	13.75	9.20

For the input data without noise the heat-transfer coefficient is reconstructed very well, irrespective of the number of the control points. Small errors are a consequence of the acceptance of the moment of the end of the numerical procedure. For the biggest number of the control points, in the case of minimization in the set V_α^0, an increase in the errors in the input data, causes an increase of the error in reconstruction of the heat-transfer coefficient, but at all times it is smaller than the errors in the input data. However, for smaller number of the control points these errors increase quickly together with an increase in the error in the input data. The improvement of the results (see Table 4) may be obtained if, instead of designating the minimum of the functional in set V_α^0, we will designate this minimum in set V_α^p for adequately selected (for example for the sake of technology) intervals $[p_{1i}, p_{2i}]$.

5.2. Three-phase problems

Example 3

In this example we will present the solution of one-dimensional three-phase problem, in which

domain Ω is interval (0,0.1) [m]. In the example we assumed the following values of the parameters used in the expression of the problem: $\lambda_1 = 54$ [W/(m · K)], $\lambda_2 = 42$ [W/(m · K)], $\lambda_3 = 30$ [W/(m · K)], $c_1 = 840$ [J/(kg · K)], $c_2 = 754$ [J/(kg · K)], $c_3 = 668$ [J/(kg · K)], $\varrho_1 = 7000$ [kg/m^3], $\varrho_2 = 7250$ [kg/m^3], $\varrho_3 = 7500$ [kg/m^3], $L_{12} = 197600$ [J/kg], $L_{23} = 49400$ [J/kg], $T^*_{12} = 1801$ [K],], $T^*_{23} = 1781$ [K], $T_\infty = 303$ [K] and the initial temperature is equal to $\varphi_0(x) = 1853$ [K]. Five points of the change in the value of the heat-transfer coefficient were assumed: $t_{\alpha 1} = 38$ [s], $t_{\alpha 2} = 180$ [s], $t_{\alpha 3} = 262$ [s], $t_{\alpha 4} = 453$ [s], $t_{\alpha 5} = 669$ [s] $t^* = 764$ [s]. The exact value of the heat-transfer coefficient is equal to:

$$\alpha(t) = \begin{cases} 1200 & \text{for } t \in [0, t_{\alpha_1}], \\ 950 & \text{for } t \in (t_{\alpha_1}, t_{\alpha_2}], \\ 600 & \text{for } t \in (t_{\alpha 2}, t_{\alpha_3}], \\ 400 & \text{for } t \in (t_{\alpha_3}, t_{\alpha_4}], \\ 300 & \text{for } t \in (t_{\alpha_4}, t_{\alpha_5}], \\ 250 & \text{for } t \in (t_{\alpha_5}, t^*). \end{cases} \tag{30}$$

TABLE 5

Absolute values of percentage relative errors in the calculations of the heat-transfer coefficient for different starting points and different number of control points

M	α_{m1}	α_{m2}	α_{m3}	α_{m4}	α_{m5}	α_{m6}
α_p = (1200,900,350,350,350,250)						
775	0.42	0.00	0.83	1.25	1.00	1.20
155	0.50	0.11	0.83	6.00	2.00	5.20
78	0.67	0.32	0.33	6.75	2.33	7.20
15	1.08	1.05	2.33	8.50	1.67	8.80
α_p = (1100,850,700,700,275,225)						
775	0.00	0.11	0.83	1.75	1.00	1.60
155	0.00	0.21	1.83	5.75	1.00	3.20
78	0.75	0.53	1.83	6.25	1.00	3.20
15	0.42	0.63	3.17	7.25	1.67	2.00
α_p = (700,700,300,300,250,200)						
775	0.00	0.21	1.00	1.50	1.33	1.60
155	0.42	0.11	1.00	5.50	1.67	3.20
78	1.08	0.53	1.17	4.75	1.67	4.80
15	0.92	1.58	0.83	7.75	1.67	5.20

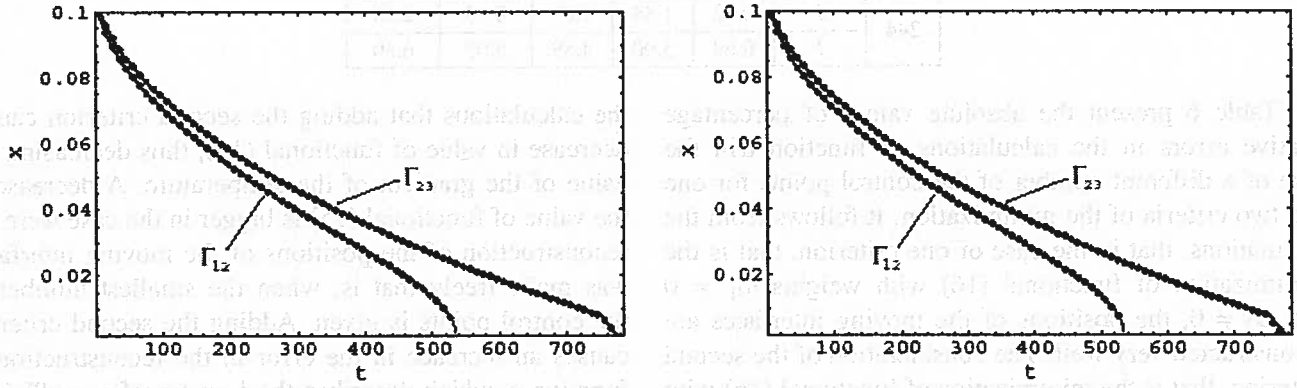

Fig. 3. Position of the moving interfaces reconstructed for $\alpha_p = (1200, 900, 350, 350, 350, 250)$ (left figure – $M = 755$, right figure – $M = 15$, solid line – exact positions, dot line – reconstructed positions)

The moving interfaces $\Gamma 12$ and Γ_{23} are given in the discrete form, for different number of the control points ($M \in \{775, 155, 78, 15\}$). The calculations were carried out for different starting points.

Table 5 present the absolute values of percentage relative errors in calculating of function α in the case of a different number of the control points and different starting points. The obtained results confirm that the

choice of the starting point for the optimization method does not have on essential influence on the value of the found point of the minimum. However, a decrease in the number of the control points causes an increase in the errors in the reconstruction of the function describing the heat-transfer coefficient.

Figure 3 presents the exact positions of the moving interfaces and positions reconstructed for the calculated point of minimum (α_m) for different starting point and different number of the control points. It follows, that the choice of the starting point and number of the control points don't have a big influence on the reconstruction of the positions of the moving interfaces.

Example 4

This example presents the solution of the axisymetrical three-phase problem, in which domain Ω is interval (0,0.6) [m]. In the example we assumed the following values of the parameters used in the expression of the problem: $\lambda_1 = 54$ [W/(m · K)], $\lambda_2 = 42$ [W/(m · K)], $\lambda_3 = 30$ [W/(m · K)], $c_1 = 840$ [J/(kg · K)], $c_2 = 754$ [J/(kg · K)], $c_3 = 668$ [J/(kg · K)], $\varrho_1 = 7000$ [kg/m^3], $\varrho_2 = 7250$ [kg/m^3], $\varrho_3 = 7500$ [kg/m^3], $L_{12} = 217600$ [J/kg], $L_{23} = 54400$ [J/kg], $T^*_{12} = 1773$ [K], $T^*_{23} = 1718$ [K], $T_\infty = 303$ [K], and the initial temperature is equal to $\varphi_0(x) = 1803$ [K]. The ends of the zones are in points: $t_{\alpha 1} = 0.4$ [s], $t_{\alpha 2} = 1.4$ [s], $t_{\alpha 3} = 2.2$ [s], $t_{\alpha 4} = 3.4$ [s], $t^* = 10$ [s].

The moving interfaces are given in the discrete form for different number of the control points ($M \in \{244, 122, 49\}$). All calculations have been carried out for the starting point $(\alpha_1, \alpha_2, \alpha_3, \alpha_4, \alpha_5) = (1450,950,650,550,270)$. The minimum of functional (16) is designated in set V^p_α:

$$V^p_\alpha = \{\alpha \in V_\alpha; \alpha_1 \in [1300, 1600] \wedge \alpha_2 \in [800, 1000] \wedge \wedge \alpha_3 \in [600, 800] \wedge \alpha_4 \in [400, 600] \wedge \alpha_1 \in [200, 300]\}.$$

The exact value of the heat-transfer coefficient is equal to:

$$\alpha(t) = \begin{cases} 1460 & \text{for } t \in [0, t_{\alpha_1}], \\ 872 & \text{for } t \in (t_{\alpha_1}, t_{\alpha_2}], \\ 695 & \text{for } t \in (t_{\alpha_2}, t_{\alpha_3}], \\ 515 & \text{for } t \in (t_{\alpha_3}, t_{\alpha_4}], \\ 250 & \text{for } t \in (t_{\alpha_4}, t^*). \end{cases} \tag{31}$$

TABLE 6

Absolute values of percentage relative errors in the calculations of the heat-transfer coefficient for different number of the control points and one and two criteria of the minimization

M	Func.	α_{m1}	α_{m2}	α_{m3}	α_{m4}	α_{m5}
49	J	4.66	2.64	6.48	5.83	2.40
	I	2.33	3.44	9.35	11.85	16.40
122	J	5.48	3.21	5.47	8.35	4.00
	I	6.51	3.67	4.75	13.20	14.40
244	J	0.62	1.84	1.87	0.19	2.00
	I	0.69	3.90	4.89	5.05	6.40

Table 6 present the absolute values of percentage relative errors in the calculations of function αin the case of a different number of the control points for one and two criteria of the minimization. It follows from the calculations, that in the case of one criterion, that is the minimization of functional (16) with weights $\omega_1 \neq 0$ and $\omega_2 \neq 0$, the positions of the moving interfaces are reconstructed very well. The consideration of the second criterion, that is the minimization of functional (16) with weights $\omega_1 \neq 0$ and $\omega_1 \neq 0$, causes extended time of the solidification. This is caused by decreasing gradient of the temperature in the solid zone. In the rows marked by letter J value of the point of minimum for the minimization of one criterion is presented. Whereas, in the rows marked by letter I the value of the point of minimum for the minimization of a two criteria. It follows from the calculations that adding the second criterion causes decrease in value of functional (15), thus decreasing the value of the gradient of the temperature. A decrease in the value of functional (15) is bigger in the case were the reconstruction of the positions of the moving interfaces was made freely that is, when the smallest number of the control points is given. Adding the second criterion causes an increace in the error in the reconstruction of function α which describes the heat-transfer coefficient. A decrease in gradient of the temperature in the solid zone to the value derived from the minimization of the two criteria, doesn't have any influence on the reconstructed position of the moving interface Γ_{12}. However, it evolves a change in the reconstructed positions of the moving interface Γ_{23}, characterized by extended time of solidification. The deviation of curve Γ_{23} from given po-

sition increases together with a decrease in the number of the control points. In the case of the biggest number of the control points, the differences between the exact and reconstruction positions of the moving interfaces are very small.

6. Conclusion

The discussed method used the Nelder-Mead optimization method and method for solving the direct Stefan problem. In the examples presented in the paper we used the generalized alternating phase truncation method (one of several tested) for the sake of its exactness and practical character in multi-phase and multi-dimensional problems.

The optimization method enables the reconstruction of the boundary condition, when the positions of the moving interfaces are well-known. This method requires the sought boundary condition to be described by means of the finite number of parameters. However, it doesn't require the sought boundary condition to be linearly dependent on these parameters. Because this method requires only function evaluations, not derivatives, the functional can also depend nonlinearly on the sought parameter. In the paper the authors presented examples of the selection of the heat-transfer coefficient in some fixed zones. Finely, the problem can be reversed, to select the number and length of the zones for fixed value of the heat-transfer coefficient.

The derived calculations show that for the input data without noise the function describing the heat-transfer coefficient is reconstructed with minimal errors, which are a consequence of the acceptance the moment of the end of the numerical procedure. For the exact input data a sensible choice of the starting point for the optimization method doesn't have an essential influence on the errors in the reconstructed the heat-transfer coefficient. A decrease in the number of the control points, for the input data without noise, doesn't cause significant changes in the reconstructed boundary condition.

The obtained results confirm the independence of the results from the random set of the perturbation. They also indicate, that for the errors not bigger than 15% the errors in the results generally don't exceed the errors in the input data. In some examples, this tendency also occurred for the errors reaching 20%. The introduction of the weight coefficients does not have a big influence on the improvement of the obtained results, when the errors in the input data are smaller than 15%. However, they significantly improve the obtained results for bigger errors.

A decrease in number of the control points causes an increase in the errors in the reconstruction of the function describing the heat-transfer coefficient, this tendency especially intensifies together with an increase in the errors in the input data.

If the solution is determined in set V_α^0, then, for big errors, the results are significantly different from the expectations. In this case, the improvement is obtained by seeking the minimum in set V_α^0 and not V_α^p, for adequately selected (for example for the sake of technology) intervals $[p_{1i}, p_{2i}]$.

The advantage of the presented method is a possibility of adding other criteria of minimization. This possibility has a special importance in the design problems, in which we want the solidification process to proceed in a given way and the finished ingot to have suitable parameters (for example no have cracks).

The presented method can be easily applied for solution of various kind of design problems, for example in designing the installation of the continuous casting (for example: selection of length of the zones in the secondary cooling region (water-spray cooling), numbers of nozzles in individual zones).

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