JOURNAL OF THEORETICAL
AND APPLIED MECHANICS
46, 2, pp. 257-268, Warsaw 2008

IDENTIFICATION OF SUBSTITUTE THERMAL CAPACITY OF SOLIDIFYING ALLOY

Ewa Majchrzak

Silesian University of Technology, Gliwice, Poland

e-mail: ewa.majchrzak@polsl.pl

Bohdan Mochnacki

Czestochowa University of Technology, Czestochowa, Poland

e-mail: moch@imi.pcz.pl

Józef S. Suchy

AGH University of Science and Technology, Cracow, Poland

e-mail: jsuchy@agh.edu.pl

In the paper, the problem of identification of substitute thermal capacity $C(T)$ is discussed. This parameter appears in the case of modelling of the solidification process on the basis of one domain approach (fixed domain method). Substitute thermal capacity (STC) can be approximated, among others, by a staircase function and this case is considered. So, it is assumed that in the mathematical model describing thermal processes in the system considered the parameters of STC are unknown. On the basis of additional information concerning the cooling (heating) curves at a selected set of points, the unknown parameters can be found. The inverse problem is solved by using the least squares criterion, in which the sensitivity coefficients are applied. On the stage of numerical simulation, the boundary element method is used. In the final part of the paper, examples of computations are shown.

Key words: casting solidification, inverse problem, numerical methods

1. Introduction

An inverse problem from the scope of thermal theory of foundry processes is discussed. The problem belongs to the group of parametric ones. From the mathematical point of view, a transient non-linear boundary-initial inverse task concerning non-homogeneous domains (casting and mould) is considered. Thermal parameters appearing in the Fourier-Kirchhoff equation corresponding to the casting area (substitute thermal capacity and thermal conductivity) are temperature-dependent, and they are assumed in the form of piece-vice constant functions. Successive 'stairs' of functions determine thermophysical parameters of the molten metal, the mushy zone and the solid body.

The introduction of substitute thermal capacity (STC) to the mathematical model of solidification and cooling processes proceeding in the casting domain leads to the model called "a one domain method" (Mochnacki and Suchy, 1995; Majchrzak and Mochnacki, 1995; Majchrzak and Szopa, 2001), because the energy equation concerns an artificially homogeneous object, while in reality, it is a composition of three time-dependent sub-domains. The substitute thermal capacity of the molten metal ($T > T_L$) and the solid body ($T < T_S$), where T_S and T_L are the border temperatures resulting from the equilibrium diagram, corresponds to volumetric specific heat, while for $[T_S, T_L]$, it is a sum of the mushy zone volumetric specific heat and the spectral latent heat controlling the solidification process (Mochnacki and Suchy, 1995; Kapturkiewicz, 2003). The aim of investigations presented in this paper is simultaneous identification of all 'stairs' determining the course of STC.

Many theoretical and experimental methods for measuring thermophysical properties have been developed in literature, they include, among others, the steady state method, the probe method, the periodic heating method, the pulse heating method, etc. However, all the above methods belong to either steady-state or constant parameters estimation. Typical simultaneous solutions concern, as a rule, the identification of several thermophysical or boundary parameters treated as constant values (e.g. Huang and Wu, 1995; Kurpisz and Nowak, 1995; Yang, 1999; Ozisik and Orlande, 1999; Abou Khachfe and Jarny, 2001). The transient function estimation is an inverse heat conduction problem, which has never been examined in the open literature from the scope of thermal theory of foundry processes.

2. Governing equations

The energy equation describing the casting solidification has the following form (Mochnacki and Suchy, 1995; Majchrzak and Mochnacki, 1995)

$$c(T)\frac{\partial T(x,t)}{\partial t} = \nabla[\lambda(T)\nabla T(x,t)] + L\frac{\partial f_S(x,t)}{\partial t} \tag{2.1}$$

where $c(T)$ is a volumetric specific heat, $\lambda(T)$ is a thermal conductivity, L is a volumetric latent heat, f_S is a volumetric solid state fraction at a considered point from the casting domain, T, x, t denote temperature, geometrical coordinates and time, respectively. The form of equation (2.1) shows that only conductional heat transfer is considered and the convection in the molten metal subdomain is neglected. The considered equation is supplemented by the equation (or equations) concerning the mould subdomain

$$c_m(T)\frac{\partial T_m(x,t)}{\partial t} = \nabla[\lambda_m(T)\nabla T_m(x,t)] \tag{2.2}$$

where c_m is the mould volumetric specific heat and λ_m is the mould thermal conductivity. In the case of typical sand moulds, on the contact surface between the casting and mould the continuity condition in the form

$$\begin{aligned} -\lambda\frac{\partial T(x,t)}{\partial n} &= -\lambda_m\frac{\partial T_m(x,t)}{\partial n} \\ T(x,t) &= T_m(x,t) \end{aligned} \tag{2.3}$$

can be accepted ($\partial/\partial n$ denotes the normal derivative).

On the external surface of the system, the condition in the general form

$$\Phi\Big[T(x,t), \frac{\partial T(x,t)}{\partial n}\Big] = 0 \tag{2.4}$$

is given. For instance, on the outer surface of the mould the Robin condition

$$-\lambda_m\frac{\partial T_m(x,t)}{\partial n} = \alpha[T_m(x,t) - T_a] \tag{2.5}$$

determines the heat exchange between the mould and environment. In equation (2.5), α is the heat transfer coefficient, and T_a is the ambient temperature.

For $t = 0$, the initial condition

$$t = 0: \qquad T(x,0) = T_0(x) \qquad\qquad T_m(x,0) = T_{m0}(x) \tag{2.6}$$

is also known.

It should be pointed out that equation (2.1) constitutes a base for the numerical modelling of solidification both in the macro (Mochnacki and Suchy, 1995; Majchrzak and Mochnacki, 1995) and the micro/macro scale (Kapturkiewicz, 2003; Majchrzak *et al.*, 2006).

In the case of a typical macro model of alloy solidification, the knowledge of temperature-dependent function f_S in the mushy zone $T \in [T_S, T_L]$ sub-domain is assumed, and then

$$\frac{\partial f_s(x,t)}{\partial t} = \frac{df_s}{dT}\frac{\partial T(x,t)}{\partial t} \tag{2.7}$$

Finally, energy equation (2.1) takes the form

$$\Big[c(T) - L\frac{df_S}{dT}\Big]\frac{\partial T(x,t)}{\partial t} = \nabla[\lambda(T)\nabla T(x,t)] \tag{2.8}$$

where

$$C(T) = c(T) - L\frac{df_S}{dT}$$

is the substitute thermal capacity. One can see that for $T > T_L : f_S = 0$, while for $T < T_S : f_S = 1$, and then $df_S/dT = 0$. So, equation (2.8) determines the thermal processes in the whole conventionally homogeneous casting domain. If the linear course of $C(T)$ for $T \in [T_S, T_L]$ is assumed, in particular a function of the form

$$f_S(T) = \frac{T_L - T(x,t)}{T_L - T_S} \tag{2.9}$$

fulfilling the conditions $f_S(T_L) = 0$, $f_S(T_S) = 1$ is taken into account, then

$$C(T) = \begin{cases} c_L & \text{for} \quad T > T_L \\ c_P + \dfrac{L}{T_L - T_S} & \text{for} \quad T_S \leqslant T \leqslant T_L \\ c_S & \text{for} \quad T < T_S \end{cases} \tag{2.10}$$

where c_L, c_S, $c_P = (c_S + c_L)/2$ are the volumetric specific heats of the molten metal, solid state and mushy zone, correspondingly. If the constant values of c_L, c_S and c_P are assumed, the substitute thermal capacity of the alloy assumes a form of the staircase function – Fig. 1. It should be pointed out that such approximation of the substitute thermal capacity is very popular and often used in computations of foundry processes.

If the solidification of pure metals or eutectic alloys is considered, it is possible to introduce an artificial mushy zone (Mochnacki and Lara, 2003) corresponding to a certain interval $T \in [T^* - \Delta T, T^* + \Delta T]$, where T^* is the solidification point, and then to define the course of f_S for the interval assumed.

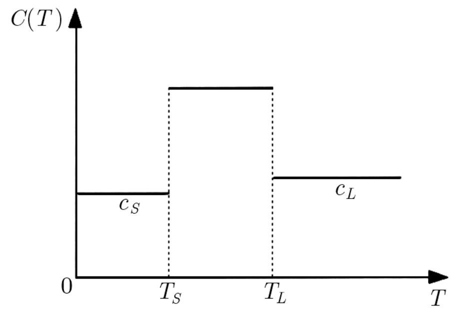

Fig. 1. Distribution of $C(T)$

3. Formulation of the inverse problem

Let us assume that the parameters appearing in the mathematical model of casing solidification are known except the segments creating the function $C(T)$. In order to solve the parametric inverse problem discussed (Kurpisz and Nowak, 1995; Ozisik and Orlande, 1999; Alifanov, 1994), it is necessary to know the values T_{gi}^f at the selected set of points x_i (sensors) from the casting-mould domain for times t^f

$$T_{gi}^f = T_g(x_i, t^f) \qquad i = 1, 2, \dots, M, \qquad f = 1, 2, \dots, F \tag{3.1}$$

For further considerations, the components of formula (2.10) are denoted in the following way

$$C(T) = \begin{cases} C_1 & \text{for} \quad T > T_L \\ C_2 & \text{for} \quad T_S \leqslant T \leqslant T_L \\ C_3 & \text{for} \quad T < T_S \end{cases} \tag{3.2}$$

and the parameters C_e, $e = 1, 2, 3$ will be estimated by using an iterative procedure.

In order to solve the inverse problem, the least squares criterion is applied

$$S(C_1, C_2, C_3) = \frac{1}{MF} \sum_{i=1}^{M} \sum_{f=1}^{F} (T_i^f - T_{gi}^f)^2 \tag{3.3}$$

where $T_i^f = T(x_i, t^f)$ are the temperatures being the solution to the direct problem for the assumed set of parameters at the points x_i, $i = 1, 2, \dots, M$ for the time t^f.

Differentiating criterion (3.3) with respect to the unknown parameters C_e and using the necessary condition of minimum, one obtains the following system of equations

$$\frac{\partial S}{\partial C_e} = \frac{2}{MF} \sum_{i=1}^{M} \sum_{f=1}^{F} (T_i^f - T_{gi}^f)(U_{ei}^f)^k = 0 \qquad e = 1,2,3 \tag{3.4}$$

where

$$(U_{ei}^f)^k = \frac{\partial T_i^f}{\partial C_e}\Big|_{C_e = C_e^k}$$

are the sensitivity coefficients, k is the number of iteration, C_e^0 are arbitrarily assumed values of C_e, while C_e^k for $k > 0$ result from the previous iteration.

The function T_i^f is expanded in the Taylor series about known values of C_l^k

$$T_i^f = (T_i^f)^k + \sum_{l=1}^{3} (U_{li}^f)^k (C_l^{k+1} - C_l^k) \tag{3.5}$$

Putting (3.5) into (3.4), one obtains $(e = 1,2,3)$

$$\sum_{i=1}^{M} \sum_{f=1}^{F} [(T_i^f)^k + \sum_{l=1}^{3} (U_{li}^f)^k (C_l^{k+1} - C_l^k) - T_{gi}^f](U_{ei}^f)^k = 0 \tag{3.6}$$

or

$$\sum_{i=1}^{M} \sum_{f=1}^{F} \sum_{l=1}^{3} (U_{li}^f)^k (U_{ei}^f)^k (C_l^{k+1} - C_l^k) = \sum_{i=1}^{M} \sum_{f=1}^{F} [T_{gi}^f - (T_i^f)^k](U_{ei}^f)^k \tag{3.7}$$

The system of equations (3.7) can be written in a matrix form

$$(\mathbf{U}^k)^\top \mathbf{U}^k \mathbf{C}^{k+1} = (\mathbf{U}^k)^\top \mathbf{U}^k \mathbf{C}^k + (\mathbf{U}^k)^\top (\mathbf{T}_g - \mathbf{T}^k) \tag{3.8}$$

where

$$\mathbf{U}^k = \begin{bmatrix} (U_{11}^1)^k & (U_{12}^1)^k & (U_{13}^1)^k \\ \cdots & \cdots & \cdots \\ (U_{11}^F)^k & (U_{12}^F)^k & (U_{13}^F)^k \\ (U_{21}^1)^k & (U_{22}^1)^k & (U_{23}^1)^k \\ \cdots & \cdots & \cdots \\ (U_{21}^F)^k & (U_{22}^F)^k & (U_{23}^F)^k \\ \cdots & \cdots & \cdots \\ (U_{M1}^1)^k & (U_{M2}^1)^k & (U_{M3}^1)^k \\ \cdots & \cdots & \cdots \\ (U_{M1}^F)^k & (U_{M2}^F)^k & (U_{M3}^F)^k \end{bmatrix} \qquad \mathbf{T}_g = \begin{bmatrix} T_{g1}^1 \\ \cdots \\ T_{g1}^F \\ T_{g2}^1 \\ \cdots \\ T_{g2}^F \\ \cdots \\ T_{gM}^1 \\ \cdots \\ T_{gM}^F \end{bmatrix} \qquad \mathbf{T}^k = \begin{bmatrix} (T_1^1)^k \\ \cdots \\ (T_1^F)^k \\ (T_2^1)^k \\ \cdots \\ (T_2^F)^k \\ \cdots \\ (T_M^1)^k \\ \cdots \\ (T_M^F)^k \end{bmatrix}$$

while

$$\mathbf{C}^k = \begin{bmatrix} C_1^k \\ C_2^k \\ C_3^k \end{bmatrix} \qquad \mathbf{C}^{k+1} = \begin{bmatrix} C_1^{k+1} \\ C_2^{k+1} \\ C_3^{k+1} \end{bmatrix} \tag{3.9}$$

This system of equations enables finding the values of C_e^{k+1}. The iteration process is stopped when the assumed number of iterations K is achieved.

It should be pointed out that in order to obtain the sensitivity coefficients, the governing equations must be differentiated with respect to C_e (direct approach – see Kleiber, 1997; Majchrzak *et al.*, 2005). So, differentiation of equation (2.8) (on the assumption that $\lambda = \text{const}$) leads to the formula

$$C(T)\frac{\partial U_e(x,t)}{\partial t} = \lambda\nabla^2 U_e(x,t) - \frac{\partial C(T)}{\partial C_e}\frac{\partial T(x,t)}{\partial t} \tag{3.10}$$

where

$$\frac{\partial C}{\partial C_1} = \begin{cases} 1 \\ 0 \\ 0 \end{cases} \qquad \frac{\partial C}{\partial C_2} = \begin{cases} 0 \\ 1 \\ 0 \end{cases} \qquad \frac{\partial C}{\partial C_3} = \begin{cases} 0 & \text{for} \quad T > T_L \\ 0 & \text{for} \quad T_S \leqslant T \leqslant T_L \\ 1 & \text{for} \quad T < T_S \end{cases}$$

The sensitivity equations for the mould ($\lambda_m = \text{const}$, $c_m = \text{const}$) subdomain have the following form

$$c_m\frac{\partial U_{me}(x,t)}{\partial t} = \lambda_m\nabla^2 U_{me}(x,t) \tag{3.11}$$

The sensitivity model is supplemented by the following conditions:
— on the contact surface

$$\begin{aligned} -\lambda\frac{\partial U_e(x,t)}{\partial n} &= -\lambda_m\frac{\partial U_{me}(x,t)}{\partial n} \\ U_e(x,t) &= U_{me}(x,t) \end{aligned} \tag{3.12}$$

— on the outer surface of the mould

$$-\lambda_m\frac{\partial U_{me}(x,t)}{\partial n} = \alpha U_{me}(x,t) \tag{3.13}$$

— and the initial condition

$$t = 0: \qquad U_e(x,0) = 0 \qquad U_{me}(x,0) = 0 \tag{3.14}$$

So, for each time step, the basic problem and three additional problems connected with the sensitivity functions should be solved.

4. Example of computations

The recurrent fragment of steel casting shown in Fig. 2 (Majchrzak and Szopa, 2001) has been considered (in particular, the symmetrical part of the domain has been taken into account).

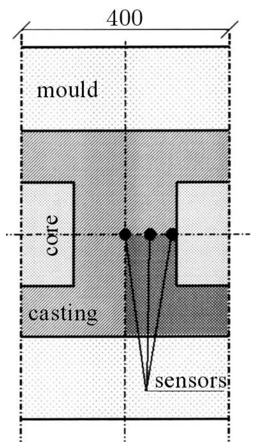

Fig. 2. Considered domain

The following thermophysical parameters of subdomains have been introduced: casting domain λ = const = 35 W/(mK), c_S = 4.875 MJ/(m^{3}K), c_L = 5.904 MJ/(m^{3}K), L = 1984.5 MJ/m^3, T_S = 1470°C, T_L = 1505°C, T_0 = 1550°C, core domain λ_{m1} = 0.7 W/(mK), c_{m1} = 1.88MJ/(m^{3}K), mould domain λ_{m2} = 1.2 W/(mK), c_{m2} = 1.76 MJ/(m^{3}K) and T_{m0} = 20°C. The positions of sensors are marked in Fig. 2. Both the basic problem and the additional ones have been solved by using the boundary element method supplemented by the temperature field correction method (Majchrzak, 2001).

In Figs. 3 and 4, the temperature field and shape of the solidified part of casting after 10 and 30 minutes are shown. This solution enables determination of the set of T_{gi}^f at the selected points from the domain considered. In Fig. 5, the iteration process of identification of parameters C_e, $e = 1, 2, 3$ is marked (starting point $C_1^0 = C_2^0 = C_3^0 = 10$ MJ/(m^{3}K)). The same computations for other initial values of C_e are shown in Fig. 6 and 7.

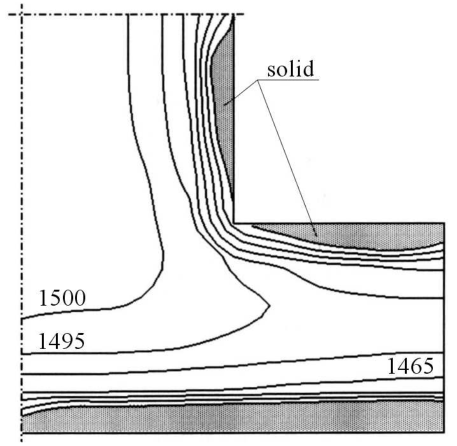

Fig. 3. Temperature distribution after 10 minutes

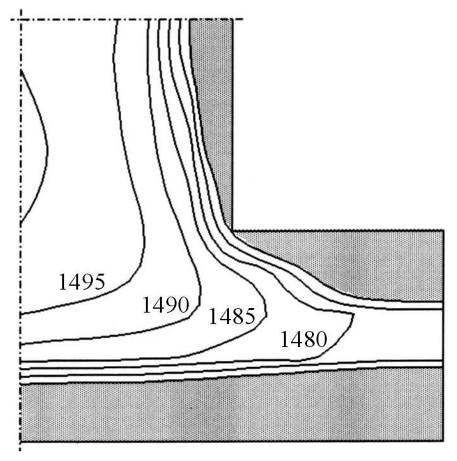

Fig. 4. Temperature distribution after 30 minutes

5. Conclusions

It should be pointed out that for the initial values assumed, the iteration process is convergent and the final values of STC are very close to the real ones. The information concerning T_{gi}^{f} and resulting from the basic problem solution was undisturbed, but similar inverse problems were also solved (Mochnacki and Metelski, 2005) by using the 'measured temperatures' disturbed in a random way. It is also possible to apply the heating curves at points from the mould

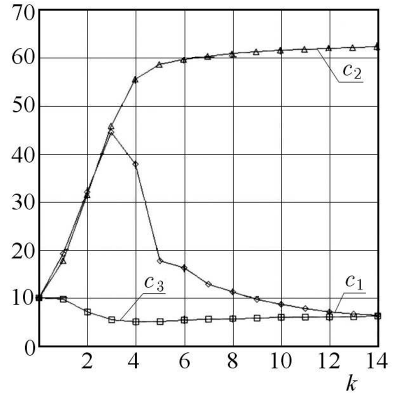

Fig. 5. Iteration process (variant I)

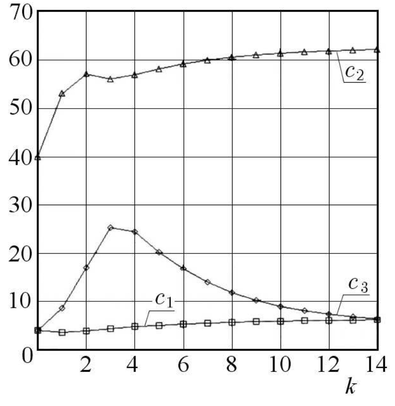

Fig. 6. Iteration process (variant II)

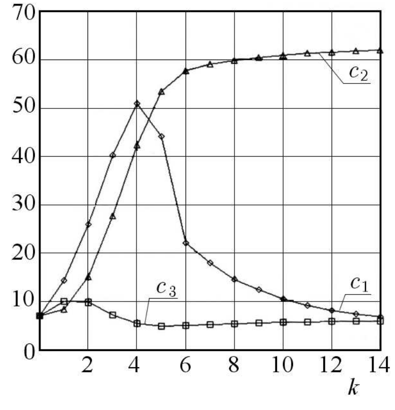

Fig. 7. Iteration process (variant III)

subdomain (Mochnacki and Majchrzak, 2006), and this information can be interesting from the practical point of view.

Summing up, the proposed approach to the solution to inverse problems seems to be an effective and simple tool for numerical analysis of heat transfer proceeding in the casting-mould system.

Acknowledgement

The paper was founded by Grant No. N507 3592 33.

References

1. ABOU KHACHFE R., JARNY Y., 2001, Determination of heat sources and heat transfer coefficient for two-dimensional heat flow – numerical and experimental study, *International Journal of Heat and Mass Transfer*, **44**, 1309-1322

2. ALIFANOV O.M., 1994, *Inverse Heat Transfer Oroblems*, Springer-Verlag, Berlin

3. HUANG C.H., WU J.Y., 1995, An inverse-problem of determining two boundary heat fluxes in unsteady heat condition of thick-walled circular cylinder, *Inverse Problems Engineering*, **1**, 133-151

4. KAPTURKIEWICZ W., 2003, *Modelling of Cast Iron Solidification*, Akapit, Cracow

5. KLEIBER M., 1997, *Parameter Sensitivity in Nonlinear Mechanics. Theory and Finite Element Computations*, J.Wiley and Sons, England

6. KURPISZ K., NOWAK A.J., 1995, *Inverse Heat Conduction*, Computational Mechanics Publications, Southampton, Boston

7. MAJCHRZAK E., 2001, *Boundary Element Method in Heat Transfer*, Publ. of the Czestochowa Univ. of Technology, Czestochowa [in Polish]

8. MAJCHRZAK E., MENDAKIEWICZ J., PIASECKA-BELKHAYAT A., 2005, Algorithm of mould thermal parameters identification in the system casting – mould-environment, *Journal of Materials Processing Technology*, **162/163**, 1544-1549

9. MAJCHRZAK E., MOCHNACKI B., 1995, Application of the BEM in the thermal theory of foundry, *Engineering Analysis with Boundary Elements*, **16**, 99-121

10. MAJCHRZAK E, SUCHY J.S., SZOPA R., 2006, Linear model of crystallization – identification of nuclei density, *Giessereiforschung, International Foundry Research*, **2**, 29-32

11. Majchrzak E., Szopa R., 2001, Analysis of thermal processes in solidifying casting using the combined variant of the BEM, *Journal of Materials Processing Technology*, **109**, 126-132
12. Mochnacki B., Lara S., 2003, The influence of artificial mushy zone parameters on the numerical solution of the Stefan problem, *Archives of Foundry*, **3**, 10, 31-36
13. Mochnacki B., Majchrzak E., 2006, The methods of inverse problems solution in the thermal theory of foundry processes, In: *Research in Polish Metallurgy at the Beginning of XXI Century*, Ed. K. Świątkowski, Committee of Metallurgy of the Polish Academy of Sciences, 239-254
14. Mochnacki B., Metelski A., 2005, Identification of internal heat source capacity in the domain of solid body, *16th International Conference on Computer Methods in Mechanics CMM-2005*, Czestochowa, Short Papers, ISBN-83-921605-2-5, 353-354
15. Mochnacki B., Suchy J.S., 1995, *Numerical Methods in Computations of Foundry Processes*, PFTA, Cracow
16. Ozisik M.N., Orlande H.R.B., 1999, *Inverse Heat Transfer: Fundamentals and Applications'*, Taylor and Francis, Pennsylvania
17. Yang C.Y., 1999, The determination of two heat sources in an inverse heat conduction problem, *International Journal of Heat and Mass Transfer*, **42**, 345-356

Identyfikacja zastępczej pojemności cieplnej krzepnącego stopu

Streszczenie

W pracy omówiono problem identyfikacji parametru nazywanego zastępczą pojemnością cieplną stopu. Zastępcza pojemność pojawia się w przypadku modelowania krzepnięcia stopów (a również czystych metali) na podstawie opisu matematycznego nazywanego metodą jednego obszaru. Przebieg tej funkcji można aproksymować na wiele sposobów, w pracy wykorzystano aproksymację funkcją kawałkami stałą. Założono, że przedmiotem identyfikacji są wartości kolejnych "schodków" tworzących pojemność zastępczą. Dodatkową informacją niezbędną do rozwiązania zadania odwrotnego są krzywe stygnięcia w wybranych punktach z obszaru krzepnącego i stygnącego metalu. Problem rozwiązano wykorzystując kryterium najmniejszych kwadratów, do którego wprowadzono współczynniki wrażliwości. Zadanie podstawowe i zadania analizy wrażliwości rozwiązano metodami numerycznymi, a w szczególności metodą elementów brzegowych. W końcowej części pracy pokazano przykład obliczeń (zadanie 2D).

Manuscript received January 30, 2007; accepted for print December 14, 2007