ARCHIVES
of
FOUNDRY ENGINEERING

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

ISSN (1897-3310)
Volume 7
Issue 4/2007

115 – 120

23/4

Shape sensitivity analysis in numerical modelling of solidification

E. Majchrzak [a, b,*], B. Mochnacki [b], G. Kałuża [a]
[a] Department for Strength of Materials and Computational Mechanics, Silesian University of Technology, Konarskiego 18a, 44-100 Gliwice, Poland
[b] Institute of Mathematics and Computer Science, Częstochowa University of Technology, Dąbrowskiego 73, 42-200 Częstochowa, Poland
*Corresponding author. E-mail address: ewa.majchrzak@polsl.pl

Received 03.07.2007; accepted in revised form 10.07.2007

Abstract

The methods of sensitivity analysis constitute a very effective tool on the stage of numerical modelling of casting solidification. It is possible, among others, to rebuilt the basic numerical solution on the solution concerning the others disturbed values of physical and geometrical parameters of the process. In this paper the problem of shape sensitivity analysis is discussed. The non-homogeneous casting-mould domain is considered and the perturbation of the solidification process due to the changes of geometrical dimensions is analyzed. From the mathematical point of view the sensitivity model is rather complex but its solution gives the interesting information concerning the mutual connections between the kinetics of casting solidification and its basic dimensions. In the final part of the paper the example of computations is shown. On the stage of numerical realization the finite difference method has been applied.

Keywords: Solidification, Numerical modelling, Inverse problem, Parameter identification

1. Introduction

The thermal processes proceeding in the casting domain are described using the one domain approach [1, 2, 3, 4], in other words, the energy equation in which substitute thermal capacity of alloy is applied. The energy equation for casting domain is supplemented by the similar equation for mould sub-domain and boundary conditions determining the heat exchange between casting and mould and on the outer surface of the mould. The initial temperatures of sub-domains are also known.

Formulated in this way boundary initial problem constitutes a basis for shape sensitivity model construction. The sensitivity equations are obtained using the direct approach [5, 6, 7] at the same time the material derivative is applied.

2. Governing equations

The casting-mould-environment system is considered. The transient temperature field in casting sub-domain is described by the following energy equation

$$(x, y) \in \Omega: \quad c(T)\frac{\partial T}{\partial t} = \nabla\left[\lambda(T)\nabla T\right] + Q \tag{1}$$

where $\lambda(T)$ is the thermal conductivity, $c(T)$ is the volumetric specific heat, $Q = Q(x, y, t)$ is the source function, $T = T(x, y, t)$, (x, y), t denote temperature, spatial co-ordinates and time, respectively.

As is well known, the source term $Q(x, y, t)$ is proportional to the local solidification rate [1, 2, 3], this means

$$Q = L\frac{\partial f_S}{\partial t} \tag{2}$$

where f_S is the solid state fraction at the neighbourhood of the point considered from casting domain, L is the volumetric latent heat.

If one assumes that f_S is the known function of temperature (the scope of f_S is from 0 to 1, of course) then

$$\frac{\partial f_S}{\partial t} = \frac{\mathrm{d} f_S}{\mathrm{d}T}\frac{\partial T}{\partial t} \tag{3}$$

and

$$(x, y) \in \Omega: \quad C(T)\frac{\partial T}{\partial t} = \nabla\left[\lambda(T)\nabla T\right] \tag{4}$$

where the parameter

$$C(T) = c(T) - L\frac{\mathrm{d} f_S}{\mathrm{d}T} \tag{5}$$

is called a substitute thermal capacity of mushy zone sub-domain [1, 2]. In the case of binary alloys the mushy zone sub-domain corresponds to the temperature interval $[T_S , T_L]$, where T_S, T_L are the border temperatures determining the end and the beginning of the solidification process.

In literature a several hypothesis concerning the function describing a substitute thermal capacity of the mushy zone are discussed [1, 3, 4]. In this paper the substitute thermal capacity for cast steel is defined as follows (Figure 1)

$$C(T) = \begin{cases} c_L, & T > T_L \\ c_1 + c_2 T + c_3 T^2 + c_4 T^3 + c_5 T^4, & T_S \le T \le T_L \\ c_S, & T < T_S \end{cases} \tag{6}$$

where c_L , c_S are the constant volumetric specific heats of liquid and solid state, c_e, $e = 1, 2, ..., 5$ are the coefficients. The coefficients c_e have been found on the basis of conditions assuring the continuity of C^1 class and physical correctness of approximation, namely

$$\begin{aligned} & C(T_L) = c_L \\ & C(T_S) = c_S \\ & \left.\frac{\mathrm{d}C(T)}{\mathrm{d}T}\right|_{T=T_L} = 0 \\ & \left.\frac{\mathrm{d}C(T)}{\mathrm{d}T}\right|_{T=T_S} = 0 \\ & \int_{T_S}^{T_L} C(T)\,\mathrm{d}T = \frac{c_S + c_L}{2}(T_L - T_S) + L \end{aligned} \tag{7}$$

Because the solidification process proceeds in a rather small interval of temperature one can assume the constant value of thermal conductivity of cast steel and then the equation (4) takes a form

$$(x, y) \in \Omega: \quad C(T)\frac{\partial T}{\partial t} = \lambda \nabla^2 T \tag{8}$$

A temperature field in mould sub-domain describes the equation of the form

$$x \in \Omega_m: \quad c_m \frac{\partial T_m(x,t)}{\partial t} = \lambda_m \nabla^2 T_m(x,t) \tag{9}$$

where λ_m and c_m are the mould thermal conductivity and the volumetric specific heat, respectively.

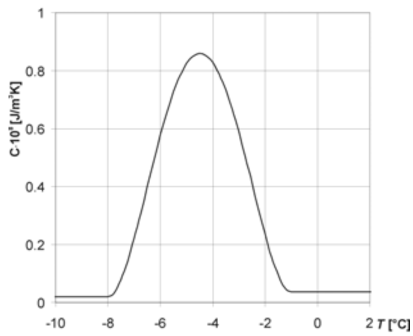

Fig. 1. Substitute thermal capacity

On the contact surface between casting and mould the continuity condition

$$(x, y) \in \Gamma_c: \quad \begin{cases} -\lambda\,\mathbf{n}\cdot\nabla T = -\lambda_m\,\mathbf{n}\cdot\nabla T_m \\ T = T_m \end{cases} \tag{10}$$

is assumed.

For the outer surface of the system the no-flux condition can be accepted

$$(x, y) \in \Gamma_0: \quad -\lambda_m\,\mathbf{n}\cdot\nabla T_m = 0 \tag{11}$$

For the moment $t = 0$ the initial temperature distribution is known, namely

$$t = 0: \; T = T_0, \quad T_m = T_{m0} \tag{12}$$

3. Shape sensitivity analysis

We assume that b is the shape design parameter. Using the concept of material derivative we can write [5, 6]

$$\frac{\mathrm{D}T}{\mathrm{D}b} = \frac{\partial T}{\partial b} + \frac{\partial T}{\partial x}v_x + \frac{\partial T}{\partial y}v_y \tag{13}$$

where $v_x = v_x(x, y, b)$ and $v_y = v_y(x, y, b)$ are the velocity associated with design parameter b.

Taking into account the definition (13) it can be proved that [8]

$$\frac{\mathrm{D}}{\mathrm{D}b}\left(\frac{\partial^2 T}{\partial x^2}\right) = \frac{\partial^2}{\partial x^2}\left(\frac{\mathrm{D}T}{\mathrm{D}b}\right) - 2\frac{\partial^2 T}{\partial x^2}\frac{\partial v_x}{\partial x} - \frac{\partial T}{\partial x}\frac{\partial^2 v_x}{\partial x^2} - 2\frac{\partial^2 T}{\partial x \partial y}\frac{\partial v_y}{\partial x} - \frac{\partial T}{\partial y}\frac{\partial^2 v_y}{\partial x^2} \tag{14}$$

and

$$\frac{\mathrm{D}}{\mathrm{D}b}\left(\frac{\partial^2 T}{\partial y^2}\right) = \frac{\partial^2}{\partial y^2}\left(\frac{\mathrm{D}T}{\mathrm{D}b}\right) - 2\frac{\partial^2 T}{\partial y^2}\frac{\partial v_y}{\partial y} - \frac{\partial T}{\partial x}\frac{\partial^2 v_x}{\partial y^2} - 2\frac{\partial^2 T}{\partial x \partial y}\frac{\partial v_x}{\partial y} - \frac{\partial T}{\partial y}\frac{\partial^2 v_y}{\partial y^2} \tag{15}$$

at the same time

$$\frac{\mathrm{D}}{\mathrm{D}b}\left(\frac{\partial T}{\partial t}\right) = \frac{\partial}{\partial t}\left(\frac{\mathrm{D}T}{\mathrm{D}b}\right) \tag{16}$$

So, for 2D domain oriented in Cartesian co-ordinate system one obtains

$$\frac{\mathrm{D}\left(\nabla^2 T\right)}{\mathrm{D}b} = \frac{\mathrm{D}}{\mathrm{D}b}\left(\frac{\partial^2 T}{\partial x^2}\right) + \frac{\mathrm{D}}{\mathrm{D}b}\left(\frac{\partial^2 T}{\partial y^2}\right) \tag{17}$$

this means

$$\frac{\mathrm{D}\left(\nabla^2 T\right)}{\mathrm{D}b} = \nabla^2\left(\frac{\mathrm{D}T}{\mathrm{D}b}\right) - 2\left(\frac{\partial^2 T}{\partial x^2}\frac{\partial v_x}{\partial x} + \frac{\partial^2 T}{\partial y^2}\frac{\partial v_y}{\partial y}\right) - \frac{\partial T}{\partial x}\left(\frac{\partial^2 v_x}{\partial x^2} + \frac{\partial^2 v_x}{\partial y^2}\right) - 2\frac{\partial^2 T}{\partial x \partial y}\left(\frac{\partial v_y}{\partial x} + \frac{\partial v_x}{\partial y}\right) - \frac{\partial T}{\partial y}\left(\frac{\partial^2 v_y}{\partial x^2} + \frac{\partial^2 v_y}{\partial y^2}\right) \tag{18}$$

It can be also proved that [5, 8]

$$\frac{\mathrm{D}\left(\mathbf{n}\cdot\nabla T\right)}{\mathrm{D}b} = \mathbf{n}\cdot\nabla\left(\frac{\mathrm{D}T}{\mathrm{D}b}\right) + \mathbf{n}\cdot\nabla T\cdot\mathbf{n}\cdot\nabla v\cdot\mathbf{n}^{\mathrm{T}} - \mathbf{n}\cdot\left[\nabla v + \left(\nabla v\right)^{\mathrm{T}}\right]\cdot\nabla T \tag{19}$$

where

$$\nabla v = \begin{bmatrix} \dfrac{\partial v_x}{\partial x} & \dfrac{\partial v_y}{\partial x} \\ \dfrac{\partial v_x}{\partial y} & \dfrac{\partial v_y}{\partial y} \end{bmatrix} \tag{20}$$

If the direct approach of sensitivity analysis is applied [5, 6, 9, 10], then the governing equations should be differentiated with respect to shape parameter b.

The differentiation of equation (8) gives

$$\frac{\mathrm{D}C\left(T\right)}{\mathrm{D}b}\frac{\partial T}{\partial t} + C\left(T\right)\frac{\partial U}{\partial t} = \lambda\nabla^2 U - 2\lambda\left(\frac{\partial^2 T}{\partial x^2}\frac{\partial v_x}{\partial x} + \frac{\partial^2 T}{\partial y^2}\frac{\partial v_y}{\partial y}\right) - \lambda\frac{\partial T}{\partial x}\left(\frac{\partial^2 v_x}{\partial x^2} + \frac{\partial^2 v_x}{\partial y^2}\right) - 2\lambda\frac{\partial^2 T}{\partial x \partial y}\left(\frac{\partial v_y}{\partial x} + \frac{\partial v_x}{\partial y}\right) - \lambda\frac{\partial T}{\partial y}\left(\frac{\partial^2 v_y}{\partial x^2} + \frac{\partial^2 v_y}{\partial y^2}\right) \tag{21}$$

where $U = \mathrm{D}T/\mathrm{D}b$ and (c.f. Fig. 2)

$$\frac{\mathrm{D}C\left(T\right)}{\mathrm{D}b} = \frac{\mathrm{d}C\left(T\right)}{\mathrm{d}T}\frac{\mathrm{D}T}{\mathrm{D}b} = \frac{\mathrm{d}C\left(T\right)}{\mathrm{d}T}U \tag{22}$$

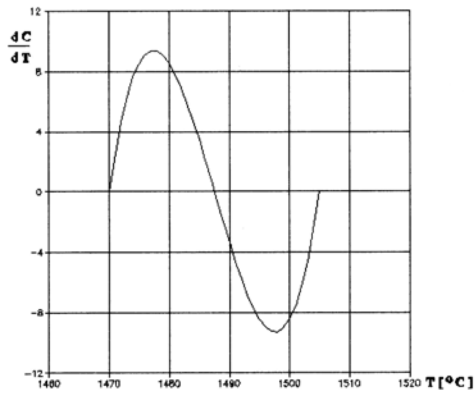

Fig. 2. Function $\mathrm{d}C(T)/\mathrm{d}T$ [MJ/m^{3}K^2]

In similar way the equation (9) is differentiated with respect to b and then

$$c_m\frac{\partial U_m}{\partial t} = \lambda_m\nabla^2 U_m - 2\lambda_m\left(\frac{\partial^2 T_m}{\partial x^2}\frac{\partial v_x}{\partial x} + \frac{\partial^2 T_m}{\partial y^2}\frac{\partial v_y}{\partial y}\right) - \lambda_m\frac{\partial T_m}{\partial x}\left(\frac{\partial^2 v_x}{\partial x^2} + \frac{\partial^2 v_x}{\partial y^2}\right) - 2\lambda_m\frac{\partial^2 T_m}{\partial x \partial y}\left(\frac{\partial v_y}{\partial x} + \frac{\partial v_x}{\partial y}\right) - \lambda_m\frac{\partial T_m}{\partial y}\left(\frac{\partial^2 v_y}{\partial x^2} + \frac{\partial^2 v_y}{\partial y^2}\right) \tag{23}$$

where $U_m = \mathrm{D}T_m/\mathrm{D}b$.

Differentiation of continuity condition (10) leads to the formula

$$\left(x, y\right)\in\Gamma_c: \quad \begin{cases} -\lambda\dfrac{\mathrm{D}\left(\mathbf{n}\cdot\nabla T\right)}{\mathrm{D}b} = -\lambda_m\dfrac{\mathrm{D}\left(\mathbf{n}\cdot\nabla T_m\right)}{\mathrm{D}b} \\ \dfrac{\mathrm{D}T}{\mathrm{D}b} = \dfrac{\mathrm{D}T_m}{\mathrm{D}b} \end{cases} \tag{24}$$

this means

$$\begin{cases} -\lambda\left\{\mathbf{n}\cdot\nabla U+\mathbf{n}\cdot\nabla T\cdot\mathbf{n}\cdot\nabla v\cdot\mathbf{n}^{\mathrm{T}}-\mathbf{n}\cdot\left[\nabla v+(\nabla v)^{\mathrm{T}}\right]\cdot\nabla T\right\}= \\ -\lambda_m\left\{\mathbf{n}\cdot\nabla U_m+\mathbf{n}\cdot\nabla T_m\cdot\mathbf{n}\cdot\nabla v\cdot\mathbf{n}^{\mathrm{T}}-\mathbf{n}\cdot\left[\nabla v+(\nabla v)^{\mathrm{T}}\right]\cdot\nabla T_m\right\} \\ U=U_m \end{cases} \quad (25)$$

The conditions (11), (12) are also differentiated with respect to b, namely

$$(x,y)\in\Gamma_0:\quad -\lambda_m\left\{\mathbf{n}\cdot\nabla U_m+\mathbf{n}\cdot\nabla T_m\cdot\mathbf{n}\cdot\nabla v\cdot\mathbf{n}^{\mathrm{T}}-\mathbf{n}\cdot\left[\nabla v+(\nabla v)^{\mathrm{T}}\right]\cdot\nabla T_m\right\}=0 \quad (26)$$

and

$$t=0:\ U=0,\qquad U_m=0 \quad (27)$$

It should be pointed out that in order to solve the additional problem connected with sensitivity functions U and U_m (equations (21)-(27)), the values of v_x, v_y should be known.

4. Shape design parameter

The cross-section of casting-mould in the form of square of dimensions $d\times d$ has been considered. It is assumed that the shape parameter b corresponds to the half of square diagonal (c.f. Figure 3) and $v_x=x/b$, $v_y=y/b$.

In this case the equation (21) takes a form

$$C(T)\frac{\partial U}{\partial t}=\lambda\nabla^2 U-\frac{2\lambda}{b}\nabla^2 T-\frac{\mathrm{d}C(T)}{\mathrm{d}T}U\frac{\partial T}{\partial t} \quad (28)$$

or (c.f. equation (8))

$$C(T)\frac{\partial U}{\partial t}=\lambda\nabla^2 U-\frac{2}{b}C(T)\frac{\partial T}{\partial t}-\frac{\mathrm{d}C(T)}{\mathrm{d}T}U\frac{\partial T}{\partial t} \quad (29)$$

The equation (23) can be written as follows

$$c_m\frac{\partial U_m}{\partial t}=\lambda_m\nabla^2 U_m-\frac{2\lambda_m}{b}\nabla^2 T_m \quad (30)$$

or (c.f. equation (9))

$$c_m\frac{\partial U_m}{\partial t}=\lambda_m\nabla^2 U_m-\frac{2}{b}c_m\frac{\partial T_m}{\partial t} \quad (31)$$

Because (c.f. formula (20))

$$\nabla v=\begin{bmatrix}\frac{1}{b} & 0\\ 0 & \frac{1}{b}\end{bmatrix}=\frac{1}{b}\mathbf{I} \quad (32)$$

so the condition (25) has a form

$$\begin{cases} -\lambda\left(\mathbf{n}\cdot\nabla U-\frac{1}{b}\mathbf{n}\cdot\nabla T\right)=-\lambda_m\left(\mathbf{n}\cdot\nabla U_m-\frac{1}{b}\mathbf{n}\cdot\nabla T_m\right) \\ U=U_m \end{cases} \quad (33)$$

or taking into account the dependence (10)

$$(x,y)\in\Gamma_c:\quad \begin{cases} -\lambda\,\mathbf{n}\cdot\nabla U=-\lambda_m\,\mathbf{n}\cdot\nabla U_m \\ U=U_m \end{cases} \quad (34)$$

while the condition (26) can be expressed as

$$(x,y)\in\Gamma_0:\quad -\lambda_m\left(\mathbf{n}\cdot\nabla U_m-\frac{1}{b}\mathbf{n}\cdot\nabla T_m\right)=0 \quad (35)$$

or (c.f. equation (11))

$$(x,y)\in\Gamma_0:\quad -\lambda_m\,\mathbf{n}\cdot\nabla U_m=0 \quad (36)$$

It should be pointed out that the additional problem above presented is coupled with the basic problem because in order to solve it, the values of $\partial T/\partial t$ and $\partial T_m/\partial t$ should be known.

5. Results of computations

The casting-mould system shown in Figure 3 has been considered. The following input data have been introduced: $\lambda = 30$ [W/(mK)], $\lambda_m = 1$ [W/(mK)], c_S = 4.875 [MJ/m^3 K], c_L = 5.904 [MJ/m^3 K], c_m = 1.75 [MJ/m^3], L = 1984.5 [MJ/m^3], pouring temperature T_0 = 1550 $^\circ$C, liquidus temperature T_L = 1505 $^\circ$C, solidus temperature T_S = 1470 $^\circ$C, initial mould temperature T_{m0} = 20 $^\circ$C.

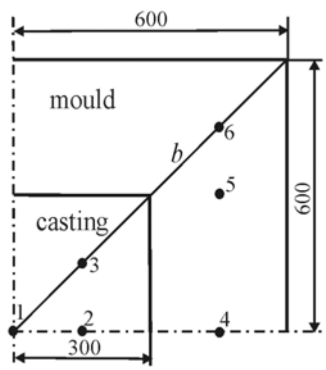

Fig. 3. Casting-mould system

The direct problem and additional one connected with the sensitivity function have been solved by means of the explicit scheme of finite difference method [1]. The regular mesh created by 30×30 nodes with constant step $h = 0.002$ [m] has been introduced, time step $\Delta t = 0.1$ [s].

In Figures 4 and 5 the distribution of temperature and function U in casting sub-domain for time 60 and 180 [s] is shown.

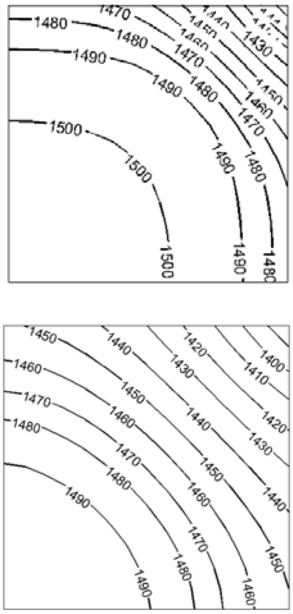

Fig. 4. Temperature distribution for time 60 and 180 [s]

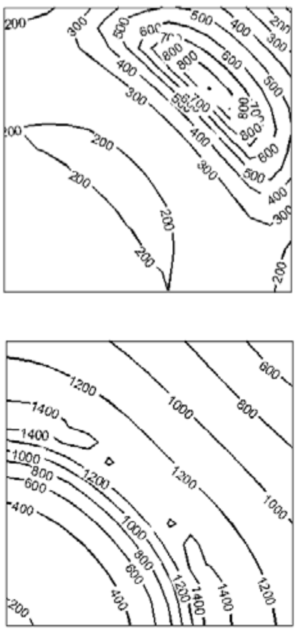

Fig. 5. Distribution of function U for time 60 and 180 [s]

Figures 6 and 7 illustrate the cooling curves and the courses of function U at the points 1, 2, 3 from casting domain marked in Figure 3.

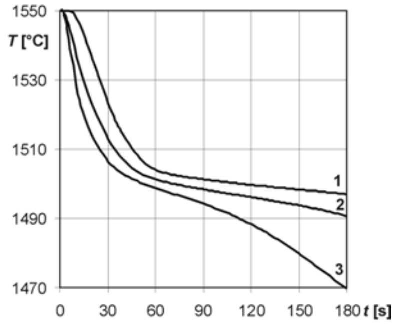

Fig. 6. Cooling curves at the points 1, 2, 3

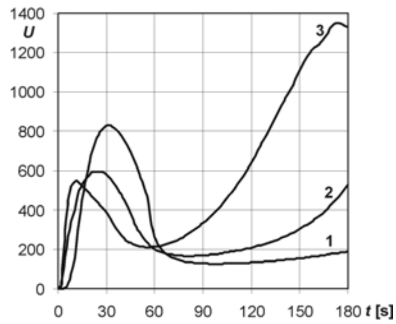

Fig. 7. Courses of sensitivity function at the points 1, 2, 3

In Figures 8 and 9 the courses of heating curves and function U at the points 4, 5, 6 from mould sub-domain marked in Figure 3 are shown.

On the basis of the knowledge of temperature T and sensitivity function U for time t and shape parameter b, the temperature in the domain for $b + \Delta b$ can be obtained using the Taylor formula

$$T(x, y, b + \Delta b, t) = T(x, y, b, t) + U(x, y, b, t)\Delta b \tag{37}$$

In Figures 10 and 11 the temperature courses at the points selected from casting and mould sub-domains for basic value of shape parameter and for $b + \Delta b$ ($\Delta b = 0.05b$) are shown.

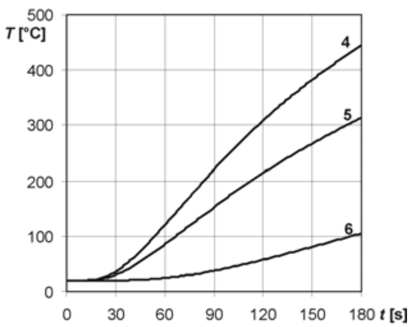

Fig. 8. Heating curves at the points 4, 5, 6

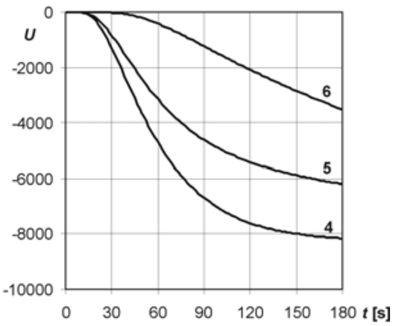

Fig. 9. Courses of sensitivity function at the points 4, 5, 6

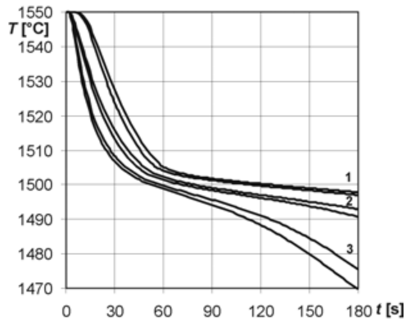

Fig. 10. Cooling curves for *b* and *b* + 0.05*b*

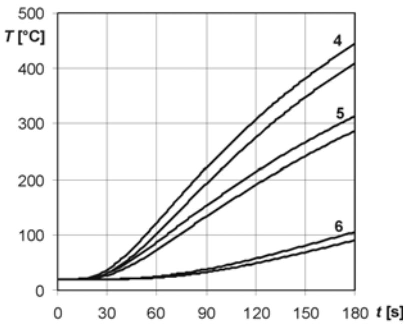

Fig. 11. Heating curves for *b* and *b* + 0.05*b*

6. Conclusions

Shape sensitivity analysis is the very effective tool in numerical modelling of solidification problem. It allows to rebuilt the basic solution on the solution concerning the other disturbed value of shape parameter. In the paper the direct approach has been presented but it is possible to use the adjoint method of shape sensitivity analysis.

References

[1] B. Mochnacki, J. S. Suchy, Numerical methods in computations of foundry processes, PFTA, Cracow, 1995.

[2] E. Majchrzak, B. Mochnacki, Identification of thermal properties of the system casting - mould, Materials Science Forum 539-543 (2007) 2491-2496.

[3] B. Mochnacki, J. S. Suchy, Identification of alloy latent heat on the basis of mould temperature (Part 1), Archives of Foundry 6, 22 (2006) 324-330.

[4] J. Mendakiewicz, Influence of choice of cast iron substitute thermal capacity on the results of numerical computations, Archives of Foundry, 6, 22 (2006) 310-315 (in Polish).

[5] M. Kleiber, Parameter sensitivity, J.Wiley & Sons Ltd., Chichester, 1997.

[6] K. Dems, B. Rousselet, Sensitivity analysis for transient heat conduction in a solid body, Structural Optimization, 17 (1999), 36-45.

[7] A. Służalec, M. Kleiber, Shape sensitivity analysis for nonlinear steady-state heat conduction problems, International Journal of Heat and Mass Transfer, Vol. 39, No 12 (1996), 2609-2613.

[8] G. Kałuża, Application of sensitivity analysis methods in bio-heat transfer, Doctoral Theses, Silesian University of Technology, Gliwice, 2005.

[9] E. Majchrzak, M. Jasiński, G. Kałuża, Application of shape sensitivity analysis in numerical modelling of solidification process, Archives of Foundry, 5, 15 (2005), 259-264.

[10] R. Szopa, The parametric sensitivity analysis of solidification process, Archives of Foundry 5, 15 (2005) 395-404.