INVERSE PROBLEMS IN THE THERMAL THEORY OF FOUNDRY PROCESSES

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Abstract. In the paper the applications of inverse problems in the thermal theory of foundry processes are discussed. Both the macro models of solidification (in particular the fixed domain approach) and macro/micro ones are considered. The information necessary in order to determine the unknown parameters of the process results from the knowledge of cooling (heating) curves at the selected set of points from casting and/or mould subdomains. The identified values can correspond to the thermophysical parameters of casting and mould, parameters appearing in boundary conditions and initial temperatures. In the paper the newest results obtained in this scope by the authors are presented. The examples of numerical solutions are also shown.

1. Mathematical formulation of direct problems

The energy equation describing the casting solidification is of the following form [1, 2]

$$c(T)\frac{\partial T(x,t)}{\partial t} = \nabla\left[\lambda(T)\,\nabla T(x,t)\right] + L\frac{\partial f_S(x,t)}{\partial t} \qquad (1)$$

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 the considered point from casting domain, T, x, t denote the temperature, geometrical co-ordinates and time. One can see that only conductional heat transfer is considered and the convection in the molten metal is neglected. The equation concerning a mould sub-domain is simpler than (1), namely

$$c_m(T)\frac{\partial T_m(x,t)}{\partial t} = \nabla\left[\lambda_m(T)\,\nabla T_m(x,t)\right] \qquad (2)$$

where c_m is a mould volumetric specific heat, λ_m is a mould thermal conductivity. In the case of typical sand molds on the contact surface casting-mould the continuity of temperature and heat flux can be accepted

$$
\begin{cases}
-\lambda \dfrac{\partial T(x, t)}{\partial n} = -\lambda_m \dfrac{\partial T_m(x, t)}{\partial n} \\[2mm]
T(x, t) = T_m(x, t)
\end{cases}
\tag{3}
$$

where $\partial/\partial n$ denotes a normal derivative.

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

$$
\Phi\left[T(x, t), \frac{\partial T(x, t)}{\partial n} \right] = 0
\tag{4}
$$

is given. In particular the typical formula determining the heat exchange between mould and environment is the following

$$
-\lambda_m \frac{\partial T_m(x, t)}{\partial n} = \alpha\left[T_m(x, t) - T_a \right]
\tag{5}
$$

where α is a heat transfer coefficient, T_α is an ambient temperature. For time $t = 0$ the initial values are also known

$$
t = 0: \quad T(x, 0) = T_0(x), \quad T_m(x, 0) = T_{m0}(x)
\tag{6}
$$

It should be pointed out that the equation (1) constitutes a base for the numerical modeling of solidification both in the macro (e.g. [1]) and the micro/macro scale (e.g. [3, 4]).

In the case of macro model (the one domain approach [1, 2, 10] is considered), one assumes the knowledge of temperature-dependent function f_S in the mushy zone $T \in [T_S, T_L]$ sub-domain and then

$$
\frac{\partial f_S(x, t)}{\partial t} = \frac{d f_S}{d T} \frac{\partial T(x, t)}{\partial t}
\tag{7}
$$

Finally the equation (1) takes a form

$$
\left[c(T) - L \frac{d f_S}{d T} \right] \frac{\partial T(x, t)}{\partial t} = \nabla\left[\lambda(T) \nabla T(x, t) \right]
\tag{8}
$$

The expression in brackets is called a substitute thermal capacity $C(T)$ [1].

One can see that for molten metal and solid body $f_S = 0$ and $f_S = 1$ correspondingly, and then $d f_S/d T = 0$. Summing up, the equation (8) describes the thermal processes in the whole, conventionally homogeneous, casting domain.

For instance, the function fulfilling the above formulated conditions can be assumed in the form

$$f_S(T) = \left(\frac{T_L - T}{T_L - T_S} \right)^n \tag{9}$$

then

$$\frac{\mathrm{d}\, f_s(T)}{\mathrm{d}\, T} = -\frac{n}{T_L - T_S} \left(\frac{T_L - T}{T_L - T_S} \right)^{n-1} \tag{10}$$

and finally

$$C(T) = c_P + \frac{L}{T_L - T_S}\, n \left(\frac{T_L - T}{T_L - T_S} \right)^{n-1} \tag{11}$$

where c_P is the mushy zone volumetric specific heat. The quotient $L/(T_L - T_S) = c_{sp}$ is called the spectral volumetric specific heat. So we can write the last formula in the form

$$C(T) = c_P + c_{sp}\, n \left(\frac{T_L - T}{T_L - T_S} \right)^{n-1} \tag{12}$$

It is easy to check that

$$\int_{T_S}^{T_L} \left[c_P + c_{sp}\, n \left(\frac{T_L - T}{T_L - T_S} \right)^{n-1} \right] \mathrm{d}T = c_P (T_L - T_S) + L \tag{13}$$

and this result confirms the proper approximation of $C(T)$. The value of exponent n can be chosen on the basis of adequate experiments. Very popular and often quoted in literature is the case concerning $n = 1$. Then

$$C(T) = c_P + \frac{L}{T_L - T_S} = c_P + c_{sp}, \quad T \in [T_S,\, T_L] \tag{14}$$

In literature one can find also the 'direct' definitions of $C(T)$, in other words the form of function $C(T)$ is assumed a'priori, for example [5]

$$C(T) = c_S + (c_{\max} - c_S) \frac{T - T_S}{T_L - T_S}, \quad T \in [T_S,\, T_L] \tag{15}$$

where c_S is a volumetric specific heat of solid, while $c_{\max}$ can be found on the basis of condition

$$\int_{T_S}^{T_L} C(T)\,\mathrm{d}T = c_P\left(T_L - T_S\right) + L \tag{16}$$

The example concerning the identification of parameters appearing in formula (16) has been shown in [5].

If one considers the solidification of pure metals or eutectic alloys then it is possible to introduce the artificial mushy zone corresponding to a certain interval $T \in \left[T^* - \Delta T,\ T^* + \Delta T\right]$, where T^* is a solidification point, and next to define the course of f_S for the interval assumed [2].

The energy equation (1) can be used also in the case of micro/macro approach to solidification process. In the group of models here discussed [3, 4, 6] we introduce the following function (in order to simplify the further considerations the solidification of pure metals or eutectic alloys is discussed, the generalized micro/macro model is presented, among others, in [7])

$$\omega(x,\,t) = N(x,\,t)\ V(x,\,t) \tag{17}$$

where N is a grains density [grains/m^3], V is a single grain volume. If we consider the spherical grains and $u = \partial R/\partial t$ is a crystallization rate (R is a grain radius) then

$$V(x,\,t) = \frac{4}{3}\pi\left[\int_0^t u(\tau)\,\mathrm{d}\tau\right]^3 \tag{18}$$

In the case of the others types of crystallization (e.g. dendritic growth) the coefficient $\nu < 1$ can be introduced [4] and then

$$V(x,\,t) = \frac{4}{3}\pi\nu\left[\int_0^t u(\tau)\,\mathrm{d}\tau\right]^3 \tag{19}$$

Finally

$$\omega(x,\,t) = \frac{4}{3}\pi\nu\,N(x,\,t)\left[\int_0^t u(\tau)\,\mathrm{d}\tau\right]^3 \tag{20}$$

In the case of so-called linear model the function f_S is assumed to be equal $\omega(x,t)$

$$f_S(x,\,t) = N(x,\,t)\ V(x,\,t) \tag{21}$$

and if $f_S = 1$ then the crystallization process stops. The derivative of f_S with respect to time equals

$$\frac{\partial f_s(x, t)}{\partial t} = 4\pi v \left[\frac{R(x, t)^3}{3} \frac{\partial N(x, t)}{\partial t} + R(x, t)^2 \frac{\partial R(x, t)}{\partial t} N(x, t) \right] \qquad (22)$$

One can see that equation (21) determines the geometrical volume (volume fraction) and it is the correct assumption on the first stages of crystallization. In order to take into account the geometrical limitations of spherical growth in the final stages of the process the equation (22) is also modified to the form

$$\frac{\partial f_s}{\partial t} = 4\pi v \left[\frac{R^3}{3} \frac{\partial N}{\partial t} + R^2 \frac{\partial R}{\partial t} N \right] (1 - f_s) \qquad (23)$$

The exponential model resulting from the theory proposed by Mehl, Johnson, Avrami and Kolmogoroff (e.g. [3, 4]) bases on the following formula

$$f_S(x, t) = 1 - \exp[-\omega(x, t)] = 1 - \exp\left\{ -\frac{4}{3}\pi v N(x, t) \left[\int_0^t dR(x, t) \right]^3 \right\} \qquad (24)$$

in other words the expression of type (17) corresponds to the exponent in equation (24). For the small geometrical volumes $\exp(-\omega) = 1 - \omega$ and the formulas (21), (24) are the same.

Additionally considering the group of models here discussed it is assumed that:

i) a local and temporary number of nuclei is proportional to the second power of undercooling below the solidification point T^*

$$N(x, t) = \eta \Delta T(x, t)^2 = \eta \left[T^* - T(x, t) \right]^2 \qquad (25)$$

where η is a nucleation coefficient. The nucleation stops when $\Delta T(x, t + \Delta t) < \Delta T(x, t)$, for $T(x, t) > T^*$: $N(x, t) = 0$.

ii) the nuclei growth is determined by the formula

$$\frac{dR(x, t)}{dt} = \mu \Delta T^m(x, t) \qquad (26)$$

where μ is the growth coefficient, $m \in [1, \ 2]$ (see [3, 8]). One can find also the other equation, namely

$$u(x, t) = \frac{dR(x, t)}{dt} = \mu_1 \Delta T(x, t)^2 + \mu_2 \Delta T(x, t)^3 \qquad (27)$$

where μ_1, μ_2 are the growth coefficients.

The interesting modification of Mehl-Johnson-Avrami-Kolmogoroff approach can be found in [8, 9].

2. Sensitivity analysis

The methods of inverse problems solution discussed in this paper require the formulation of sensitivity models with respect to physical, boundary or initial parameters (in particular the so-called sensitivity coefficients must be determined). The sensitivity of temperature with respect to parameter p_k is defined in the following way [10]

$$U_k\left(x,t,p_1^0,...,p_n^0\right) = \lim_{\Delta p_k \to 0} \frac{T\left(x,t,p_1^0,...,p_k^0+\Delta p_k,...,p_n^0\right)-T\left(x,t,p_1^0,...,p_k^0,...,p_n^0\right)}{\Delta p_k}$$

(28)

and it corresponds to the partial derivative of temperature with respect to p_k. So the sensitivity function informs about the changes of temperature due to changes of p_k. The definition (28) is often used in practical applications because the knowledge of two solutions corresponding to the small changes of p_k allows (using the differential quotient) to determine the local values of sensitivity. More general approach to the computations of sensitivity function consists in the differentiation of the basic equation and conditions with respect to the parameter analyzed (direct approach [10]).

Below the sensitivity of temperature field in the system casting mould with respect to mould parameters c_m, λ_m, boundary parameters α, T_a or initial ones $\left(T_0, T_{m0}\right)$ will be discussed. At first, the energy equation (8) for casting domain will be differentiated with respect to p_k

$$\frac{\partial}{\partial p_k}\left[C(T)\frac{\partial T(x,t)}{\partial t}\right] = \nabla\left[\frac{\partial}{\partial p_k}\left[\lambda(T)\nabla T(x,t)\right]\right]$$

(29)

After the mathematical manipulations one obtains

$$C(T)\frac{\partial U(x,t)}{\partial t} = \nabla\left[\lambda(T)\nabla U(x,t)\right]+\nabla\left[\frac{d\lambda(T)}{dT}U(x,t)\nabla T(x,t)\right]$$
$$-\frac{dC(T)}{dT}U(x,t)\frac{\partial T(x,t)}{\partial t}$$

(30)

where $U = \partial T/\partial p_k$.

For the mould sub-domain (assuming the constant values of c_m, λ_m)

$$c_m\frac{\partial U_m(x,t)}{\partial t} = \lambda_m\nabla^2 U_m(x,t)+\left(\frac{\partial \lambda_m}{\partial p_k}\frac{c_m}{\lambda_m}-\frac{\partial c_m}{\partial p_k}\right)\frac{\partial T_m(x,t)}{\partial t}$$

(31)

where $U_m = \partial T_m / \partial p_k$. The Robin condition (5) leads to the formula

$$-\frac{\partial \lambda_m}{\partial p_k} \frac{\partial T_m(x,t)}{\partial n} - \lambda_m \frac{\partial U_m(x,t)}{\partial n} = \frac{\partial \alpha}{\partial p_k}\left[T_m(x,t) - T_a\right] + \alpha\left[U_m(x,t) - \frac{\partial T_a}{\partial p_k}\right] \quad (32)$$

while the continuity condition (3) on the contact surface takes a form

$$\begin{cases} -\dfrac{\mathrm{d}\lambda(T)}{\mathrm{d}t} U(x,t) \dfrac{\partial T(x,t)}{\partial n} - \lambda(T)\dfrac{\partial U(x,t)}{\partial n} = -\dfrac{\partial \lambda_m}{\partial p_k}\dfrac{\partial T_m(x,t)}{\partial n} - \lambda_m \dfrac{\partial U_m(x,t)}{\partial n} \\[2mm] \qquad\qquad\qquad U(x,t) = U_m(x,t) \end{cases}$$

$$(33)$$

The sensitivity model is supplemented by the initial conditions

$$t = 0: \qquad U(x,0) = U_0, \quad U_m(x,0) = U_{m0} \qquad (34)$$

If the sensitivity analysis does not concern the initial temperatures then the conditions (34) are uniform (zero-ones). It should be pointed out that the sensitivity equations are essentially simpler if one considers the actual parameter p_k. Additionally the assumption that the thermal conductivity λ is a constant value or piece-wise constant function leads to the simpler form of sensitivity model.

In the second part of this chapter, as an example of micro/macro approach will be presented. In particular, the sensitivity of solidification process described by the Kolmogoroff model with respect to the mould thermal conductivity λ_m will be discussed. The construction of sensitivity models with respect to others parameters is similar, of course. Assuming the constant number of nuclei (nuclei density) we obtain the following form of exponent in equation (24)

$$\omega(x,t) = \frac{4}{3}\pi v N\left[\int_0^t u(\tau)\,\mathrm{d}\tau\right]^3 \qquad (35)$$

while the nuclei growth is assumed to be determined by the formula

$$u(x,t) = \frac{\partial R(x,t)}{\partial t} = \mu\,\Delta T(x,t) \qquad (36)$$

which corresponds to exponent $m = 1$ (c.f. (26)). For $c(T) = c = $ const and $\lambda(T) = \lambda = $ const (taking into account the small interval of temperature in which the essential phenomena connected with solidification proceed, such assumption is quite acceptable) the energy equation (1) takes a form

$$c\frac{\partial T(x,t)}{\partial t} = \lambda \nabla^2 T(x,t) + L\exp[-\omega(x,t)]\frac{\partial \omega(x,t)}{\partial t} \qquad (37)$$

or

$$c\frac{\partial T}{\partial t} = \lambda\nabla^2 T + 4\pi\nu NL\mu\Delta T\left(\int_0^t \mu\Delta T\,\mathrm{d}\tau\right)^2 \exp\left[-\frac{4}{3}\pi\nu N\left(\int_0^t \mu\Delta T\,\mathrm{d}\tau\right)^3\right] \quad (38)$$

According to the rules of direct approach the equations determining the thermal processes in the system casting mould should be differentiated with respect to λ_m and then

$$\begin{cases} x\in\Omega: & c\frac{\partial U(x,t)}{\partial t} = \lambda\nabla^2 U(x,t)+Q \\[2mm] x\in\Omega_m: & c_m\frac{\partial U_m(x,t)}{\partial t} = \lambda_m\nabla^2 U_m(x,t)+\frac{c_m}{\lambda_m}\frac{\partial T_m(x,t)}{\partial t} \\[2mm] x\in\Gamma_m: & \begin{cases} U(x,t)=U_m(x,t) \\[2mm] -\lambda\frac{\partial U(x,t)}{\partial n} = -\frac{\partial T_m(x,t)}{\partial n}-\lambda_m\frac{\partial U_m(x,t)}{\partial n} \end{cases} \\[2mm] x\in\Gamma_0: & -\lambda_m\frac{\partial U_m(x,t)}{\partial n} = \alpha U_m(x,t)+\frac{\partial T_m(x,t)}{\partial n} \\[2mm] t=0: & U(x,0)=0, \quad U_m(x,0)=0 \end{cases} \quad (39)$$

where Ω, Ω_m, Γ_m, Γ_0 denote the casting and mould sub-domains, the contact and outer surface of mould, correspondingly.

The function Q in equation concerning the casting volume results from the differentiation of source term in (38) with respect to λ_m

$$Q = \frac{\partial}{\partial\lambda_m}\left\{4\pi\nu NL\mu\Delta T\left(\int_0^t \mu\Delta T\,\mathrm{d}\tau\right)^2 \exp\left[-\frac{4}{3}\pi\nu N\left(\int_0^t \mu\Delta T\,\mathrm{d}\tau\right)^3\right]\right\} \quad (40)$$

and we obtain (for $\nu=1$)

$$Q = 4\pi NL\exp\left(-\frac{4}{3}\pi N r_S^3\right)\left[4\pi N\mu\Delta T\rho_S r_S^4 - 2\mu\Delta T\rho_S r_S - \mu U_1 r_S^2\right] \quad (41)$$

The last formula seems to be complicated, but on the stage of numerical simulation the computations of local values Q are rather simple.

3. Inverse problems

In order to explain the details concerning the inverse problems solution the following example will be more exactly presented [6]. We consider the linear

model of crystallization (equation (21)) and the identified parameter corresponds to the nuclei density N = const. Thermophysical parameters of casting material are constant: $\lambda(T) = \lambda$, $c(T) = c$. The influence of mould is approximated by the Robin condition given on the external surface of casting (α in condition of type (5) is a substitute heat transfer coefficient, T_a is an assumed ambient temperature).

The additional information necessary in order to solve the identification problem results from the knowledge of temperature values T_{di}^f at the selected set of points x_i from casting sub-domain for times t^f, namely

$$T_{di}^f = T_d(x_i, t^f), \qquad i = 1, 2, ..., M, \qquad f = 1, 2, ..., F \tag{42}$$

At first, the least squares criterion is applied [11-13]

$$S = \sum_{i=1}^{M} \sum_{f=1}^{F} \left(T_i^f - T_{di}^f \right)^2 \tag{43}$$

where $T_i^f = T(x_i, t^t)$ is the calculated temperature at the point x_i for time t^f for arbitrary assumed value of N, $T_{di}^f = T_d(x_i, t^f)$. Differentiating the criterion (43) with respect to the unknown grains density N and using the necessary condition of minimum, one obtains

$$\frac{dS}{d\lambda} = 2 \sum_{i=1}^{M} \sum_{f=1}^{F} \left(T_i^f - T_{di}^f \right) \left. \frac{\partial T_i^f}{\partial N} \right|_{N=N^k} = 0 \tag{44}$$

at the same time N^k for $k = 0$ is an arbitrary assumed initial value of nuclei density, while for $k > 0$ N^k will result from the previous iteration step.

Function $T_i^f = T(x_i, t^t)$ is expanded into Taylor's series about known value of N^k, namely

$$T_i^f = \left(T_i^f \right)^k + \left. \frac{\partial T_i^f}{\partial N} \right|_{N=N^k} \left(N^{k+1} - N^k \right) \tag{45}$$

or

$$T_i^f = \left(T_i^f \right)^k + \left(U_i^f \right)^k \left(N^{k+1} - N^k \right) \tag{46}$$

where $\left(T_i^f \right)^k$ denotes the temperature at point x_i for time t^f found on the basis of energy equation (1) and adequate boundary-initial conditions under the assumption that N equals N^k, $\left(U_i^f \right)^k$ are the sensitivity coefficients found on the basis of sensitivity problem solution under the same assumption. So, we have

$$\sum_{i=1}^{M} \sum_{f=1}^{F} \left[\left(T_i^f\right)^k + \left(Z_i^f\right)^k \left(N^{k+1} - N^k\right) - T_{d\,i}^f \right] \left(U_i^f\right)^k = 0 \qquad (47)$$

and

$$N^{k+1} = N^k + \frac{\displaystyle\sum_{i=1}^{M} \sum_{f=1}^{F} \left[T_{d\,i}^f - \left(T_i^f\right)^k \right] \left(U_i^f\right)^k}{\displaystyle\sum_{i=1}^{M} \sum_{f=1}^{F} \left[\left(U_i^f\right)^k \right]^2}, \quad k = 0, 1, \ldots \qquad (48)$$

The estimation of parameter N is realized using the iterative procedure assuming the start point $N^0 > 0$. For every iteration step the basic problem and sensitivity one should be solved assuming $N = N^k$, and next using the equation (48) the new value $N = N^{k+1}$ can be found.

Now, let us assume that we want simultaneously identify two unknown parameters, in particular N and c (one can see that the unknown parameters belong to

the different levels of solidification process description - macro and macro/micro levels). Then the necessary condition of functional (43) minimum leads to the equations

$$\begin{cases} \dfrac{\partial S}{\partial N} = 2 \sum_{i=1}^{M} \sum_{f=1}^{F} \left(T_i^f - T_{d\,i}^f\right) \left.\dfrac{\partial T_i^f}{\partial N}\right|_{N=N^k} = 0 \\[4mm] \dfrac{\partial S}{\partial c} = 2 \sum_{i=1}^{M} \sum_{f=1}^{F} \left(T_i^f - T_{d\,i}^f\right) \left.\dfrac{\partial T_i^f}{\partial c}\right|_{c=c^k} = 0 \end{cases} \qquad (49)$$

where $T_{d\,i}^f = T_d(x_i, t^f)$, $T_i^f = T(x_i, t^f)$, N^k, c^k for $k = 0$ are the initial values (start point), while for $k > 1$ result from the previous computations. Introducing the sensitivity functions we have

$$\begin{cases} \sum_{i=1}^{M} \sum_{f=1}^{F} \left(T_i^f - T_{d\,i}^f\right) \left(U_{1i}^f\right)^k = 0 \\[4mm] \sum_{i=1}^{M} \sum_{f=1}^{F} \left(T_i^f - T_{d\,i}^f\right) \left(U_{2i}^f\right)^k = 0 \end{cases} \qquad (50)$$

where U_1 is the sensitivity with respect to N, U_2 is the sensitivity with respect to c. Now the function T_i^f is expanded into Taylor series, namely

$$T_i^f = \left(T_i^f\right)^k + \left(U_{1i}^f\right)^k \left(N^{k+1} - N^k\right) + \left(U_{2i}^f\right)^k \left(c^{k+1} - c^k\right) \tag{51}$$

Introducing (51) into (50) one obtains

$$\begin{bmatrix} \sum\limits_{i=1}^{M}\sum\limits_{f=1}^{F}\left[\left(U_{1i}^f\right)^k\right]^2 & \sum\limits_{i=1}^{M}\sum\limits_{f=1}^{F}\left(U_{1i}^f\right)^k\left(U_{2i}^f\right)^k \\ \sum\limits_{i=1}^{M}\sum\limits_{f=1}^{F}\left(U_{2i}^f\right)^k\left(U_{1i}^f\right)^k & \sum\limits_{i=1}^{M}\sum\limits_{f=1}^{F}\left[\left(U_{2i}^f\right)^k\right]^2 \end{bmatrix} \cdot \begin{bmatrix} N^{k+1} - N^k \\ c^{k+1} - c^k \end{bmatrix} =$$

$$= \begin{bmatrix} \sum\limits_{i=1}^{M}\sum\limits_{f=1}^{F}\left(U_{1i}^f\right)^k\left[T_{di}^f - \left(T_i^f\right)^k\right] \\ \sum\limits_{i=1}^{M}\sum\limits_{f=1}^{F}\left(U_{2i}^f\right)^k\left[T_{di}^f - \left(T_i^f\right)^k\right] \end{bmatrix} \tag{52}$$

This system of equations allows to determine N^{k+1} and c^{k+1}. If the iteration process is convergent then the sequences $\{N^k\}$ and $\{c^k\}$ tend towards the real values of N and c.

4. Examples of numerical solutions

The inverse problems discussed here can be solved using the numerical methods. The greater part of results presented has been obtained using the boundary element method [14, 15] though the other methods (FDM, FEM) have been also used.

The first example is very simple, but it shows the basic elements of identification problem solution. So, the following 1D boundary-initial problem is considered

$$\begin{cases} 0 < x < L: & c\,\dfrac{\partial T(x,t)}{\partial t} = \lambda\,\dfrac{\partial^2 T(x,t)}{\partial x^2} \\ x = 0: & q(x,t) = q_b \\ x = L: & q(x,t) = 0 \\ t = 0: & T(x,t) = T_0(x) \end{cases} \tag{53}$$

where L is the thickness of the plate, q_b is the known boundary heat flux, $T_0(x)$ is the initial temperature.

The direct problem described by equations (53) can be solved under the assumption that the thermophysical parameters c and λ are known. The inverse problem discussed resolves itself into identification of c on the basis of additional

information concerning cooling (heating) curves at the selected set of points from the domain considered.

At first the model of sensitivity with respect to c must be constructed. Differentiating the equation and conditions (53) with respect to c one obtains

$$
\begin{cases}
0 < x < L: & c\,\dfrac{\partial Z(x,t)}{\partial t} = \lambda\,\dfrac{\partial^2 Z(x,t)}{\partial x^2} - \dfrac{\partial T(x,t)}{\partial t} \\[2mm]
x = 0: & W(x,t) = 0 \\[1mm]
x = L: & W(x,t) = 0 \\[1mm]
t = 0: & Z(x,t) = 0
\end{cases}
\tag{54}
$$

where $Z(x,t) = \partial T(x,t)/\partial c$ and $W(x,t) = -\lambda\,\partial Z(x,t)/\partial x$. The solution of problem (54) allows to find the sensitivity coefficients appearing in the final formula (c.f. (48))

$$
c^{k+1} = c^k + \frac{\displaystyle\sum_{i=1}^{M}\sum_{f=1}^{F}\left[T_{d\,i}^{f} - \left(T_i^{f}\right)^k\right]\left(Z_i^{f}\right)^k}{\displaystyle\sum_{i=1}^{M}\sum_{f=1}^{F}\left[\left(Z_i^{f}\right)^k\right]^2}, \quad k = 0, 1, \dots
\tag{55}
$$

The sensitivity model is coupled with the basic one (term $\partial T/\partial t$) and the computations of temperature and sensitivity fields must be realized simultaneously.

The results presented below [16] concern the plate ($L = 0.02$ m, $\lambda = 1$ W/mK, $c = 10^6$ J/m^{3}K - this value is identified). The boundary heat flux equals $q_b = 3 \cdot 10^4$ W/m^2 initial temperature $T_0 = 20^{\circ}$C. The information concerning the courses of temperature at the points $x = 0$ (plate surface), $x = L/4$ and $x = L/2$ (Fig. 1) results from the solution of direct problem for $c = 10^6$ J/m^{3}K.
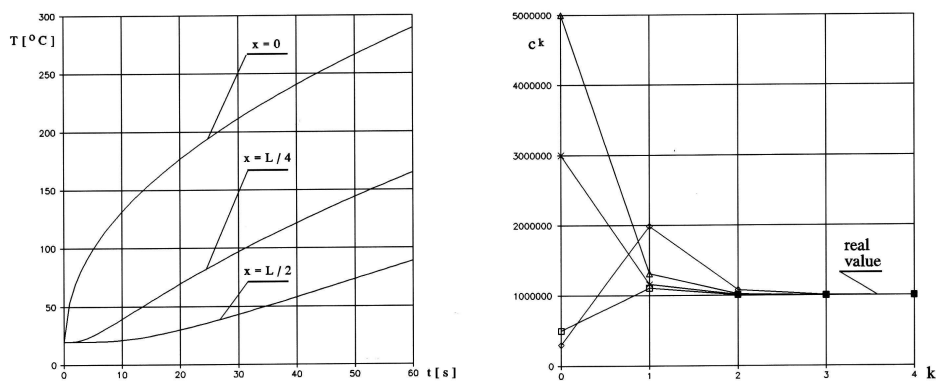
Fig. 1. Heating curves   Fig. 2. Identified volumetric specific heat

In Figure 2 the values of identified volumetric specific heat during successive iterations for different initial values c^0 are shown. It is visible, that the iteration process is quickly convergent.

The second example is more complicated and the aim of computations is the identification of latent heat [17]. The 1D casting (G = 2.4 cm) made from Al-Si alloy (5% Si) is produced in the sand mould. The parameters of casting material are equal to c_s = 2.943 MJ/m^{3}K, c_p = 3.0, c_L = 3.07, λ_S = 250 W/mK, λ_p = 177, λ_L = 104, L = 990.6 MJ/m^3 (this value is identified). The volumetric specific heat of mould c_m = 1.750 MJ/m^{3}K, while the thermal conductivity λ_m = 1.5 W/mK. Symbols L, P, S correspond to molten metal, mushy zone and solid state. Additionally it was assumed that the substitute thermal capacity of mushy zone results from formula (14). The border and initial temperatures equal T_S = 577°C, T_L = 650°C, T_0 = 660°C, T_{m0} = 20°C. On a stage of numerical modelling the finite differences method (FDM) has been used. The casting-mould domain has been divided into 100 control volumes (20 - casting, 80 - mould), time step Δt = 0.001 s. On the external surface of mould the non-flux condition has been assumed. The values of 'measured' temperatures result from the direct problem solution (for above collected input data) or this solution disturbed in random way (in order to be closer to real measurements). The parameters c_S and c_L are known, while $C(T)$ for $T \in \left[T_S, T_L \right]$ is unknown. Summing up, the following function is considered

$$C(T) = \begin{cases} 2.943 & T < 577 \\ 3.006 + \dfrac{L}{73} & T \in [577,\ 650] \\ 3.070 & T > 650 \end{cases} \qquad (56)$$

The reconstructed value of latent heat equals L = 990.6 MJ/m^3. The start point from iteration process corresponds to $c_L(L^0 = c_S)$. One can notice that distance between L^0 and real value of L is rather long.
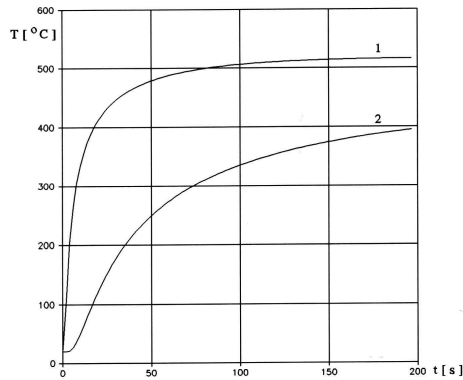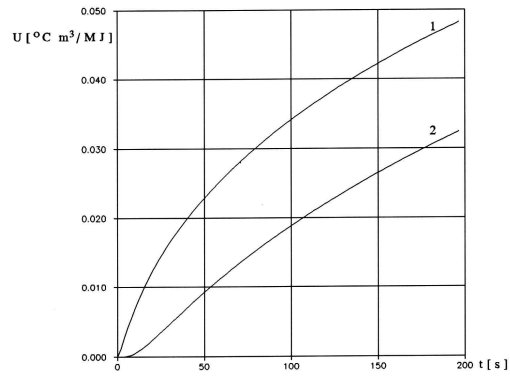
Fig. 3. Heating curves

Fig. 4. Sensitivity function (200 s)

In Figure 3 the 'measured' heating curves at points $x_1 = 1.5$ cm and $x_2 = 2$ cm found on the basis of direct problem solution for $L = 990.6$ MJ/m^3 are shown. The points x_1 and x_2 belong to the mould sub-domain. Figure 4 illustrates the distribution of sensitivity function for the final time of simulation (200 s).
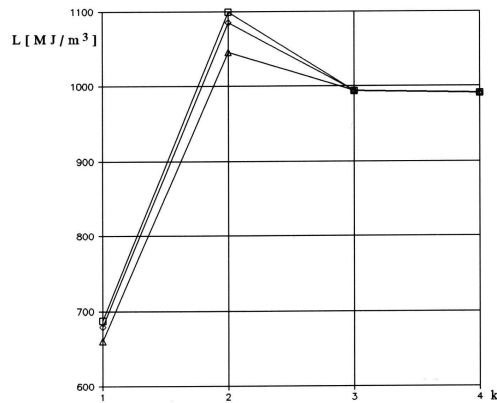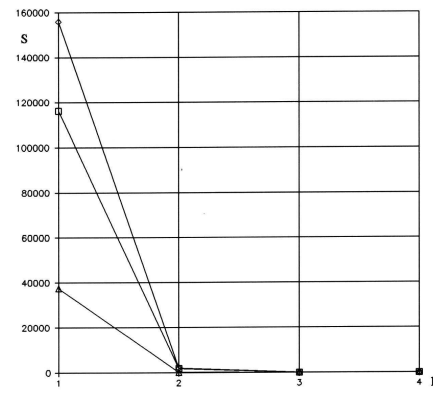
Fig. 5. Identification of latent heat

Fig. 6. Changes of criterion S

In Figure 5 the iteration process of latent heat identification is shown. The successive versions correspond to the assumptions that only the heating curve for $x_1 = 1.5$ cm is introduced to criterion (43), only the heating curve for $x_2 = 2$ cm is introduced to criterion (43) and, finally, the both curves are taken into account. Next figure shows the changes of functional S for successive iterations (the temperatures at the points $x_1 = 1.5$ cm, $x_2 = 2$ cm have been applied). It should be pointed out that the good identification has been obtained on the basis of heating curves from mould sub-domain. This information seems to be essential from

the practical point of view because the temperature measurements at this region are simple and exact.

Presented below next example concerns the macro/micro models. The aim of computations [6] was the identification of nuclei density (c.f. formula (48)), at the same time the Kolmogoroff model of crystallization is taken into account. The plate of thickness $L = 0.03$ m made from aluminium has been considered. The following input data are assumed: thermal conductivity $\lambda = 150$ W/mK, volumetric specific heat $c = 2.875 \cdot 10^6$ J/m^{3}K, latent heat per unit of volume $L = 9.75 \cdot 10^8$ J/m^3, solidification point $T^* = 660^{\circ}$C, growth coefficient $\mu = 3 \cdot 10^{-6}$ m/sK^2, initial temperature $T_p = 662^{\circ}$C, boundary temperature $T_b = 650^{\circ}$C (the influence of mould is substituted by the Dirichlet condition).

In order to estimate the value of N the courses of cooling curves at the points 1 - 0.0015 m (distance between the point and the boundary of plate), 2 - 0.0035 m and 3 - 0.0055 m have been taken into account - Figure 7. They result from the direct problem solution under the assumption that $N = 10^{10}$ nuceli/m^3. Figure 8 illustrates the solution of inverse problem for different initial values of N^0. It is visible that the iteration process is convergent and the solution close to the exact value is obtained after the several iterations. The problem has been solved using the BEM.
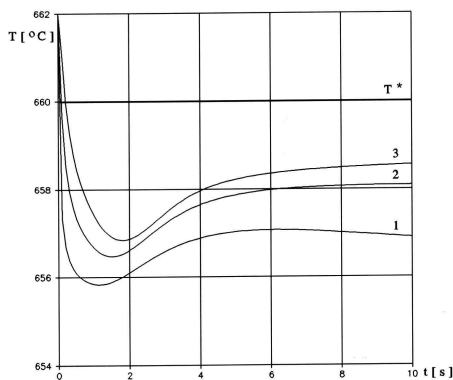

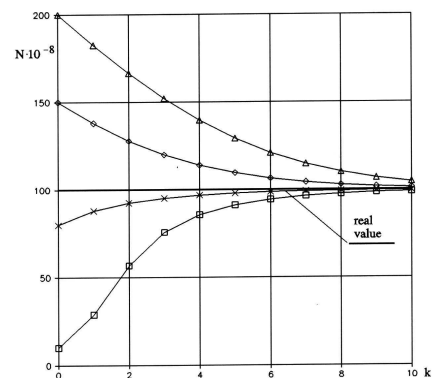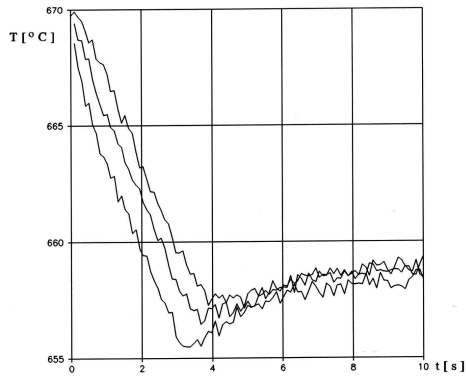Fig. 7. Cooling curves   Fig. 8. Inverse problem solution
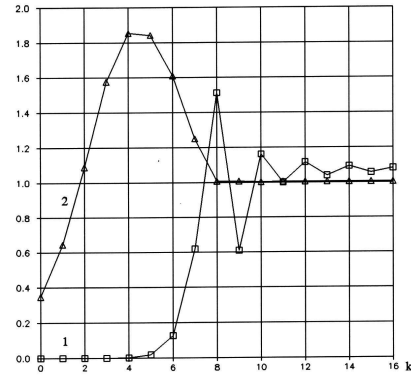
Fig. 9. Disturbed cooling curves

Fig. 10. Identification process

The last example shows the solution concerning the simultaneous identification of nuclei density and volumetric specific heat on the basis of linear model of crystallization (c.f. formula (52)). In particular the aluminium plate ($G = 3$ cm - 1D task) has been considered [18]. The influence of mould is taken into account by the Robin condition for $x = -1.5$ and $x = 1.5$ (heat transfer coefficient $\alpha = 250$ W/m^{2}K). Nuclei density $N = 10^{10}$, volumetric specific heat $c = 2.875$ MJ/m^{3}K, the others parameters of material are equal $\lambda = 150$ W/mK, $L = 975$ MJ/m^3, $\mu = 3 \cdot 10^{-6}$ m/sK^2 solidification point $T^* = 660^{\circ}$C, pouring temperature $T_0 = 670^{\circ}$C. The cooling curves $T_d \left(x_i, t^f \right)$ corresponding to the basic solution have been disturbed in random way (Fig. 9). The results of identification corresponding to successive iterations resulting from equation (52) are shown in Figure 10 ($N^0 = 1$, $c^0 = 1$). One can see that the iterative process is convergent and the final values of N and c are sufficiently exact.

Summing up, the information concerning the cooling curves at the selected set of points from casting domain allows to reconstruct parameters determining the solidification process even in the case when they belong to different (macro and micro) levels. The least squares criterion in which the sensitivity coefficients are introduced constitutes a very effective tool for numerical solution of inverse problems from the scope of thermal theory of foundry processes (the same approach has been used by the authors of this paper also in the case of others problems).

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