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Identification of solidification process parameters

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In the paper, the identification problems connected with estimation of cast iron and mould thermophysical parameters are discussed. The additional information necessary to solve the problem results from the knowledge of cooling (heating) curves at the set of points from casting (mould) domain. The course of cooling (heating) curves results from the temperature measurements done in the real conditions of technological process, but at the present stage of research the numerical solution of direct problem plays the role of measured temperatures. In this place the problem of optimal sensors position in a system casting-mould appears. Both the choice of measuring points and also the solution of inverse problem, using the gradient methods, require the application of sensitivity analysis methods. The theoretical considerations are illustrated by the examples of computations. The numerical algorithms presented base on the finite difference method (2D problems are considered).

Keywords: solidification process, numerical techniques, sensitivity analysis, inverse problems, identification methods

1. Introduction

Numerical simulation of solidification process constitutes a very effective tool for optimal design of casting production technology. Introducing to the computer program different variants of input data concerning the details of casting-mould geometry, initial temperatures, properties of mould subdomain etc., one can determine the variant of technology assuring the good quality of final product. The basis of numerical model construction results from the assumed mathematical description of the thermal processes proceeding in the system considered [1–10].

The solidification model used in this paper belongs to the group of macro ones and it is created by a system of partial differential equations (energy equations), supplemented by a set of boundary and initial conditions resulting from the technology considered. The knowledge of mathematical description of the process and the knowledge of parameters appearing in governing equation allows to solve the so-called direct problem (using, as a rule, numerical methods). In the case when one or higher number of parameters is unknown, then the inverse task should be formulated [11–19]. The additional information necessary to solve the problem results from the measured (or postulated) courses of temperature at the points selected from the casting-mould domain. At the stage of identification algorithm construction, the real measurements are replaced by a direct problem solution (or this solution disturbed in a random way). In literature one can find different methods of identification problem solutions [12, 13, 20–23]; here the gradient method basing on the least squares criterion and sensitivity coefficients has been used [12, 16, 24–29]. In the simplest version of computations only a single parameter has been identified, more complex tasks concern the simultaneous identification of the higher number of unknown parameters. At the stage of numerical modelling, the finite difference method for non-linear parabolic equations has been applied [1].

2. Direct problem

The energy equation describing the casting solidification is of the form [1, 2, 8]

$$x \in \Omega : c(T)\frac{\partial T(x,t)}{\partial t} = \nabla\Big(\lambda(T)\nabla T(x,t)\Big) + L\frac{\partial f_S(x,t)}{\partial t}, \tag{1}$$

where Ω is a casting domain, $c(T)$ 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 in the neighborhood of the point considered, T, $x = x_1, x_2$, t denote the temperature, geometrical co-ordinates and time.

If one assumes the constant value of thermal conductivity λ of casting material, then Eq. (1) can be expressed as follows

$$x \in \Omega : c(T)\frac{\partial T(x,t)}{\partial t} = \lambda\nabla^2 T(x,t) + L\frac{\partial f_S(x,t)}{\partial t}. \tag{2}$$

In the case of typical macro models (e.g. the one domain approach [1, 10, 16], one assumes the knowledge of temperature-dependent function $f_S(T)$ in the mushy zone $T \in [T_S, T_L]$ sub-domain (T_S and T_L are the temperatures corresponding to the end and beginning of alloy solidification) and then

$$\frac{\partial f_S(x,t)}{\partial t} = \frac{df_S(T)}{dT}\frac{\partial T(x,t)}{\partial t}. \tag{3}$$

So, Eq. (1) takes the form

$$x \in \Omega : C(T)\frac{\partial T(x,t)}{\partial t} = \nabla\Big(\lambda(T)\nabla T(x,t)\Big), \tag{4}$$

where

$$C(T) = c(T) - L\frac{df_S(T)}{dT} \tag{5}$$

is called a substitute thermal capacity [1, 9, 18].

It is self-evident that for molten metal and solidified part of casting $f_S = 0$, $f_S = 1$, respectively and then $df_S/dT = 0$. Summing up, Eq. (8) describes the thermal processes in the entire, conventionally homogeneous, casting domain. The substitute thermal capacity can be written in the form

$$C(T) = \begin{cases} c_L, & T > T_L, \\ c_P - L\frac{df_S(T)}{dT}, & T_S < T \le T_L, \\ c_S, & T \le T_S, \end{cases} \tag{6}$$

where c_L, c_S, $c_P = 0.5(c_L + c_S)$ are the constant volumetric specific heats of molten metal, solid state and mushy zone subdomain.

In a case of cast iron solidification, the following approximation of substitute thermal capacity can be taken into account (Fig. 1) [30, 31, 32]

$$C(T) = \begin{cases} c_L, & T > T_L, \\ \frac{c_L+c_S}{2} + \frac{Q_{aus}}{T_L-T_E}, & T_E < T \le T_L, \\ \frac{c_L+c_S}{2} + \frac{Q_{eu}}{T_E-T_S}, & T_S < T \le T_E, \\ c_S, & T \le T_S, \end{cases}, \tag{7}$$

where T_E is the temperature corresponding to the beginning of eutectic crystallization, Q_{aus}, Q_{eu} are the latent heats connected with the austenite and eutectic phases evolution. The energy equation

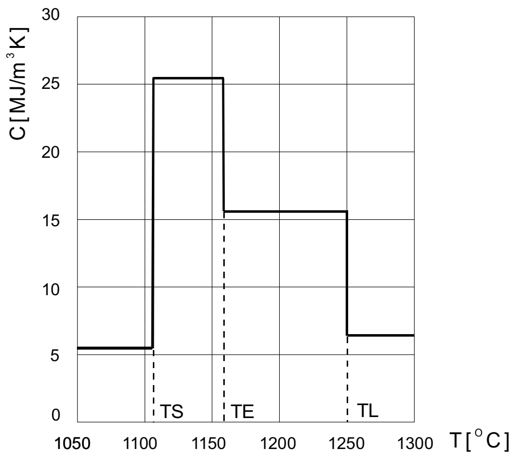

Fig. 1. Substitute thermal capacity of cast iron

concerning the casting domain is supplemented by the equation determining heat transfer processes in a mould

$$x \in \Omega_{\mathrm{m}} : c_{\mathrm{m}} \frac{\partial T_{\mathrm{m}}(x,t)}{\partial t} = \lambda_{\mathrm{m}} \nabla^2 T_{\mathrm{m}}(x,t) \tag{8}$$

where c_{m} is the mould volumetric specific heat, λ_{m} is the mould thermal conductivity (parameters c_{m}, λ_{m} are assumed to be constant).

In the case of typical sand moulds on the contact surface between casting and mould, the continuity condition in the form

$$x \in \Gamma_{\mathrm{c}} : \begin{cases} -\lambda \mathbf{n} \cdot \nabla T(x,t) = -\lambda_{\mathrm{m}} \mathbf{n} \cdot \nabla T_{\mathrm{m}}(x,t), \\ T(x,t) = T_{\mathrm{m}}(x,t) \end{cases} \tag{9}$$

can be accepted. On the external surface of the system, the Robin condition

$$x \in \Gamma_0 : -\lambda_{\mathrm{m}} \mathbf{n} \cdot \nabla T_{\mathrm{m}}(x,t) = \alpha \left(T_{\mathrm{m}}(x,t) - T_{\mathrm{a}} \right) \tag{10}$$

is given (α is the heat transfer coefficient, T_{a} is the ambient temperature).

For time $t = 0$, the initial condition

$$t = 0 : T(x,0) = T_0(x), \qquad T_{\mathrm{m}}(x,0) = T_{\mathrm{m}\,0}(x) \tag{11}$$

is also known.

As an example of direct problem solution, the thermal processes proceeding in the system, the casting-mould system shown in Fig. 2 is analyzed. To obtain the numerical solution basing on FDM, the domain considered was covered by regular mesh created by 25×15 nodes with constant step $h = 0.002$ m (Fig. 3), time step: $\Delta t = 0.1$ s (this value assures the stability of explicit differential scheme).

The following input data have been taken into account [30, 31]: $\lambda = 30\,\mathrm{W/(m\,K)}$, $\lambda_{\mathrm{m}} = 1\,\mathrm{W/(m\,K)}$, $c_{\mathrm{L}} = 5.88\,\mathrm{MJ/(m^3\ K)}$, $c_{\mathrm{S}} = 5.4\,\mathrm{MJ/(m^3\ K)}$, $Q_{\mathrm{aus}} = 923\,\mathrm{MJ/m^3}$, $Q_{\mathrm{eu}} = 994\,\mathrm{MJ/m^3}$, $c_{\mathrm{m}} = 1.75\,\mathrm{MJ/(m^3\ K)}$, pouring temperature $T_0 = 1300\,^{\circ}\mathrm{C}$, liquidus temperature $T_{\mathrm{L}} = 1250\,^{\circ}\mathrm{C}$, border temperature $T_{\mathrm{E}} = 1160\,^{\circ}\mathrm{C}$, solidus temperature $T_{\mathrm{E}} = 1110\,^{\circ}\mathrm{C}$, initial mould temperature $T_{\mathrm{m}\,0} = 20\,^{\circ}\mathrm{C}$. In Figs. 4 and 5 the temperature distributions in casting and mould for times 90 and 180 s are presented.

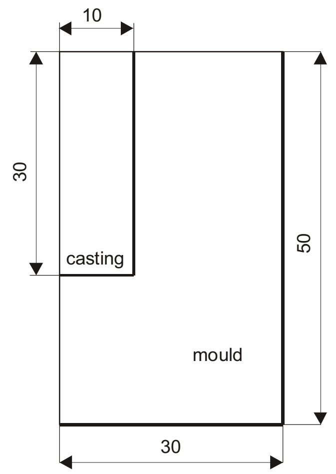

Fig. 2. Casting-mould system

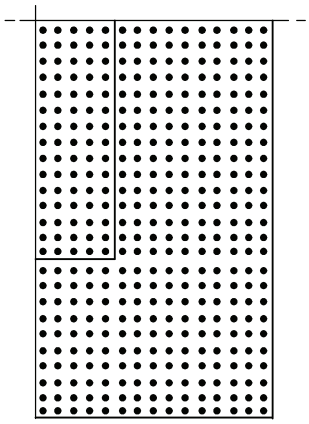

Fig. 3. Discretization

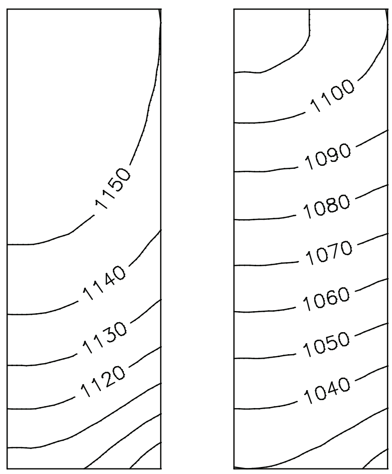

Fig. 4. Temperature distribution in casting subdomain

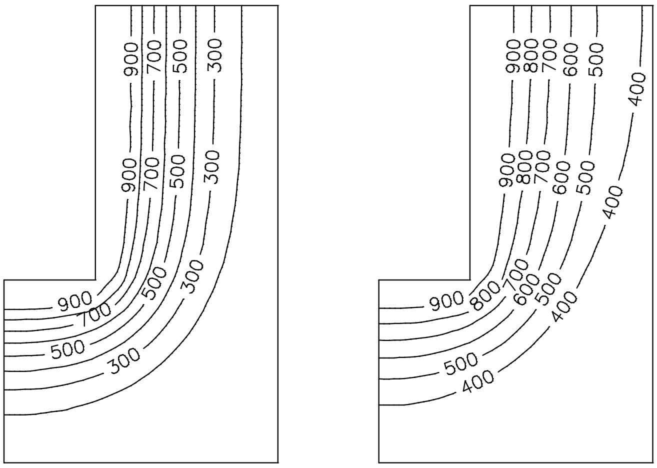

Fig. 5. Temperature distribution in mould subdomain

3. Sensitivity analysis

Sensitivity of temperature field with respect to parameter pe is defined in the following way

$$Z_e(x,t) = \lim_{\Delta p_e \to 0} \frac{T(x,t,p_1,\ldots,p_e+\Delta p_e,\ldots,p_E) - T(x,t,p_1,\ldots,p_e,\ldots,p_E)}{\Delta p_e} \tag{12}$$

this means

$$Z_e(x,t) = \frac{\partial T(x,t,p_1,\ldots,p_e,\ldots,p_{\mathrm{E}})}{\partial p_e} \tag{13}$$

The parameters p_e correspond to thermophysical properties of material (parametric sensitivity analysis), coefficients appearing in boundary conditions (e.g. heat transfer coefficient, ambient temperature), border and initial temperatures etc. The knowledge of sensitivity U_e distribution gives (among others) the information concerning the changes of local and temporary temperature due to perturbation of the parameter p_e – it results from the Taylor formula

$$T(x,t,p_1,\ldots,p_e+\Delta p_e,\ldots,p_E) = T(x,t,p_1,\ldots,p_e,\ldots,p_{\mathrm{E}}) + Z_e(x,t)\Delta p_e. \tag{14}$$

The simplest way of sensitivity models construction is the differentiation of governing equations creating the mathematical model of the process, considered with respect to distinguished parameter p_e (the direct approach [20, 25–29]).

To simplify the mathematical formulas we assume that the thermal conductivity of casting material is a constant value (c_{m} and λ_{m} are also constant) and then the differentiation of governing equations presented in the previous chapter with respect to p_e gives the following formulas

$$\begin{aligned}
&x \in \Omega : C(T)\frac{\partial Z_e(x,t)}{\partial t} = \lambda \nabla^2 Z_e(x,t) + \frac{\partial \lambda}{\partial p_e}\nabla^2 T(x,t) - \frac{\partial C(T)}{\partial p_e}\frac{\partial T(x,t)}{\partial t},\\
&x \in \Omega_{\mathrm{m}} : c_{\mathrm{m}}\frac{\partial Z_{\mathrm{m}\,e}(x,t)}{\partial t} = \lambda_{\mathrm{m}} \nabla^2 Z_{\mathrm{m}\,e}(x,t) + \frac{\partial \lambda_{\mathrm{m}}}{\partial p_e}\nabla^2 T(x,t) - \frac{\partial c_{\mathrm{m}}}{\partial p_e}\frac{\partial T_{\mathrm{m}}(x,t)}{\partial t},\\
&x \in \Gamma_{\mathrm{c}} : \begin{cases} -\lambda \mathbf{n}\cdot\nabla Z_e(x,t) = -\lambda_{\mathrm{m}}\mathbf{n}\cdot\nabla Z_{\mathrm{m}\,e}(x,t) - \dfrac{\partial \lambda_{\mathrm{m}}}{\partial p_e}\mathbf{n}\cdot T_{\mathrm{m}\,e}(x,t) + \dfrac{\partial \lambda}{\partial p_e}\mathbf{n}\cdot\nabla T(x,t), \\ Z_e(x,t) = Z_{\mathrm{m}\,e}(x,t), \end{cases}\\
&x \in \Gamma_0 : -\mathbf{n}\cdot\nabla T_{\mathrm{m}\,e}(x,t) - \lambda_{\mathrm{m}}\mathbf{n}\cdot\nabla Z_{\mathrm{m}\,e}(x,t) = \alpha\left(Z_{\mathrm{m}\,e}(x,t) - \frac{\partial T_a}{\partial p_e}\right),\\
&t = 0 : Z_e(x,0) = 0, \qquad Z_{\mathrm{m}\,e}(x,0) = 0,
\end{aligned} \tag{15}$$

where

$$Z_e(x,t) = \frac{\partial T(x,t)}{\partial p_e}, \qquad Z_{\mathrm{m}\,e}(x,t) = \frac{\partial T_{\mathrm{m}}(x,t)}{\partial p_e}. \tag{16}$$

One can see that the sensitivity model and the basic one are very close (system of two parabolic equations supplemented by the similar boundary and initial conditions). This fact is essential for numerical modelling of both problems. The sensitivity problem and the basic one are coupled and the solution concerning Z_e requires the knowledge of temperature distribution $T(x,t)$.

As an example, in Figs. 6 and 7 the distribution of sensitivity functions $\partial T/\partial\lambda_{\mathrm{m}}$ and $\partial T/\partial c_{\mathrm{m}}$ for the task discussed in the previous chapter are shown.

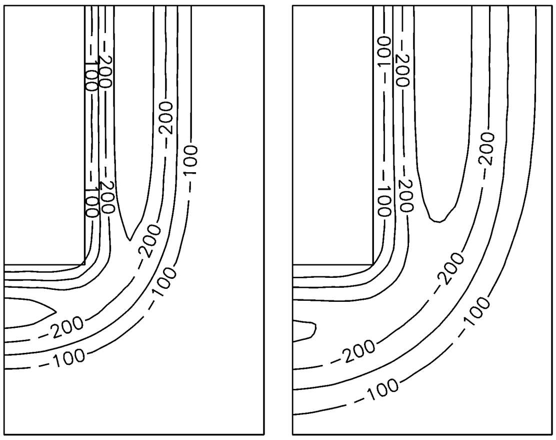

Fig. 6. Distribution of function $\partial T/\partial\lambda_{\mathrm{m}}$ for times 30 and 90 s

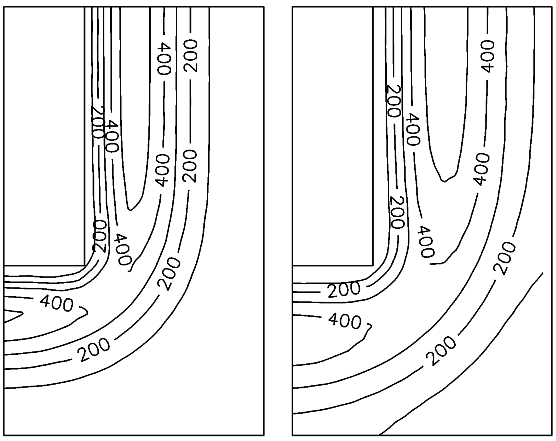

Fig. 7. Distribution of function $\partial T/\partial c_{\mathrm{m}}$ for times 30 and 90 s

4. Optimal sensors location

A fundamental problem connected with identification of the solidification parameters is the selection of sensors locations. On the one hand, the limited number of measurement points in the domain considered should be taken into account; on the other hand, the best estimators of solidification parameters are expected. Usually, the location of sensors is determined by physical conditions and by intuition. The other approach consists in application of the efficient numerical algorithms of optimum experimental design. These algorithms usually base on the Fisher Information Matrix, and A-optimality or D-optimality criterions [33–35] are generalized here to the unsteady problems.

The unknown parameters will be denoted by p_e, $e = 1, 2, \ldots, E$. For example, if the thermophysical parameters of mould should be identified, then $p_1 = \lambda_{\mathrm{m}}$ corresponds to the thermal conductivity of mould, $p_2 = c_{\mathrm{m}}$ corresponds to the mould volumetric specific heat and $E = 2$. If the aim of considerations is connected with the estimation of substitute thermal capacity (cf. Eq. 7) then $p_1 = c_{\mathrm{L}}$, $p_2 = c_{\mathrm{S}}$, $p_3 = Q_{\mathrm{eu}}$, $p_4 = Q_{\mathrm{aus}}$ and $E = 4$.

The unknown parameters can be identified on the basis of temperature measurements at the points x^i, $i = 1, 2, \ldots, M$ from casting and/or mould sub-domain:

$$T_{d\,i}^{f} = T_d(x^i, t^f), \qquad f = 1, 2, \ldots, F, \tag{17}$$

where $t^f = f\Delta t$ and Δt is the time step.

As it was mentioned above, a fundamental problem is the selection of sensors location. The additional problem is connected with determination of sufficient sensors number. It should be pointed out that the number of sensors should be greater or equal to the number of identified parameters ($M \geq E$). Majority of the methods assuring the best location of sensors (thermocouples) bases on the Fisher Information Matrix [33]. To construct this matrix in the case of unsteady heat transfer, the following sensitivity coefficients should be determined:

$$Z_{i\,e}^{f} = \frac{\partial T\left(x^i, t^f, p_1^0, \ldots, p_e^0, \ldots, p_E^0\right)}{\partial p_e^0}, \qquad e = 1, 2, \ldots, E, \tag{18}$$

where p_e^0 are the *a priori* estimates of the parameters p_e available, e.g. from the preliminary experiments.

The following matrix is constructed:

$$\mathbf{Z} = \begin{bmatrix} Z_{i\,1}^{1} & Z_{i\,2}^{1} & \ldots & Z_{i\,E}^{1} \\ Z_{i\,1}^{2} & Z_{i\,2}^{2} & \ldots & Z_{i\,E}^{2} \\ \ldots & \ldots & \ldots & \ldots \\ Z_{i\,1}^{F} & Z_{i\,2}^{F} & \ldots & Z_{i\,E}^{F} \end{bmatrix}. \tag{19}$$

It is easy to check that the product of transpose of a matrix $\mathbf{Z}^T\left(x^i\right)$ and matrix $\mathbf{Z}\left(x^i\right)$ equals

$$\mathbf{Z}^T\left(x^i\right)\mathbf{Z}\left(x^i\right) = \begin{bmatrix} \sum\limits_{f=1}^{F}\left(Z_{i\,1}^{f}\right)^2 & \sum\limits_{f=1}^{F} Z_{i\,1}^{f} Z_{i\,2}^{f} & \ldots & \sum\limits_{f=1}^{F} Z_{i\,1}^{f} Z_{i\,E}^{f} \\ \sum\limits_{f=1}^{F} Z_{i\,1}^{f} Z_{i\,2}^{f} & \sum\limits_{f=1}^{F}\left(Z_{i\,2}^{f}\right)^2 & \ldots & \sum\limits_{f=1}^{F} Z_{i\,2}^{f} Z_{i\,E}^{f} \\ \ldots & \ldots & \ldots & \ldots \\ \sum\limits_{f=1}^{F} Z_{i\,1}^{f} Z_{i\,E}^{f} & \sum\limits_{f=1}^{F} Z_{i\,2}^{f} Z_{i\,E}^{f} & \ldots & \sum\limits_{f=1}^{F}\left(Z_{i\,E}^{f}\right)^2 \end{bmatrix}. \tag{20}$$

The Fisher Information Matrix is the following [33, 35]

$$\mathbf{F}\left(w_1, w_2, \ldots, w_M\right) = \sum_{i=1}^{M} w_i \mathbf{Z}^T\left(x^i\right)\mathbf{Z}\left(x^i\right), \tag{21}$$

where $w_1, w_2, \ldots, w_M$ are the weights connected with the points x^i; additionally $0 \leq w_i \leq 1$, $i = 1, 2, \ldots, M$ and

$$\sum_{i=1}^{M} w_i = 1. \tag{22}$$

After the mathematical manipulations, the FIM takes a form

$$\mathbf{F}\left(w_1,\dots,w_m\right)=\begin{bmatrix}\sum\limits_{i=1}^{M} w_i\sum\limits_{f=1}^{F}\left(Z_{i\,1}^{f}\right)^2 & \sum\limits_{i=1}^{M} w_i\sum\limits_{f=1}^{F} Z_{i\,1}^{f}Z_{i\,2}^{f} & \dots & \sum\limits_{i=1}^{M} w_i\sum\limits_{f=1}^{F} Z_{i\,1}^{f}Z_{i\,E}^{f}\\ \sum\limits_{i=1}^{M} w_i\sum\limits_{f=1}^{F} Z_{i\,1}^{f}Z_{i\,2}^{f} & \sum\limits_{i=1}^{M} w_i\sum\limits_{f=1}^{F}\left(Z_{i\,2}^{f}\right)^2 & \dots & \sum\limits_{i=1}^{M} w_i\sum\limits_{f=1}^{F} Z_{i\,2}^{f}Z_{i\,E}^{f}\\ \dots & \dots & \dots & \dots\\ \sum\limits_{i=1}^{M} w_i\sum\limits_{f=1}^{F} Z_{i\,1}^{f}Z_{i\,E}^{f} & \sum\limits_{i=1}^{M} w_i\sum\limits_{f=1}^{F} Z_{i\,2}^{f}Z_{i\,E}^{f} & \dots & \sum\limits_{i=1}^{M} w_i\sum\limits_{f=1}^{F}\left(Z_{i\,E}^{f}\right)^2\end{bmatrix}. \tag{23}$$

Different criteria of optimality can be taken into account [33]. One of them is the A-optimality which is connected with minimization of the *trace* of information matrix (23). The other is the D-optimality criterion depending on the maximization of the *determinant* of the information matrix (23).

Using A-optimality criterion, the following problem should be solved

$$\begin{aligned}&S(w_1,w_2,\dots,w_M)=\operatorname{tr}\mathbf{F}^{-1}(w_1,w_2,\dots,w_M)\to\min,\\&0\le w_i\le 1,\qquad i=1,2,\dots,M,\\&\sum_{i=1}^{M}w_i=1.\end{aligned} \tag{24}$$

If the D-optimality criterion is applied, then the problem has the form

$$\begin{aligned}&S(w_1,w_2,\dots,w_M)=\det\mathbf{F}(w_1,w_2,\dots,w_M)\to\max,\\&0\le w_i\le 1,\qquad i=1,2,\dots,M,\\&\sum_{i=1}^{M}w_i=1.\end{aligned} \tag{25}$$

So, if we consider a set of points $X=\{x_1,x_2,\dots,x_M\}$ at which measurements may be taken, the practical design problem consists in selecting of the corresponding weights $w_1,w_2,\dots,w_M$ which define the best experimental conditions.

In the paper, a simpler algorithm (from the numerical point of view) is proposed [36, 37]. Let X denote the set of possible sensors locations $X=\{x_1,x_2,\dots,x_M\}$ and let N be the number of sensors. For each point x^i, $i=1,2,\dots,M$ the sensitivity coefficients (18) are calculated [38].

As previously, for the point considered x^i the matrix $\mathbf{Z}\left(x^i\right)$ is constructed (cf. Eq. 19).

If $\{x^{i\,1},x^{i\,2},\dots,x^{i\,N}\}$ denotes the optional subset of set X then the number of possibilities is equal to C_N^M (number of combinations without repetitions). For every combination the following matrix is defined

$$\mathbf{Z}\left(x^{i\,1},x^{i\,2},\dots,x^{i\,N}\right)=\begin{bmatrix}\mathbf{Z}\left(x^{i\,1}\right)\\ \mathbf{Z}\left(x^{i\,2}\right)\\ \mathbf{Z}\left(x^{i\,N}\right)\end{bmatrix}. \tag{26}$$

In the case considered, the Fisher Information Matrix has the form

$$\mathbf{F}\left(x^{i\,1},x^{i\,2},\dots,x^{i\,N}\right)=\mathbf{Z}^{\mathrm{T}}\left(x^{i\,1},x^{i\,2},\dots,x^{i\,N}\right)\mathbf{Z}\left(x^{i\,1},x^{i\,2},\dots,x^{i\,N}\right). \tag{27}$$

D-optimality criterion used in the design of sensors location is the following

$$\det\mathbf{F}\left(x^{i\,1^*},x^{i\,2^*},\dots,x^{i\,N^*}\right)=\max_{\left(x^{i\,1},x^{i\,2},\dots,x^{i\,N}\right)}\det\mathbf{F}\left(x^{i\,1},x^{i\,2},\dots,x^{i\,N}\right). \tag{28}$$

The points $x^{i\,1^*}, x^{i\,2^*}, \ldots, x^{i\,N^*}$ correspond to the best positions of N sensors.

The algorithm is simple but time-consuming, because a considerable number of sensitivity problems must be solved.

The first example concerns the optimal position of two sensors used for estimation of mould thermophysical parameters. The geometry of heterogeneous system casting-mould is shown in Fig. 2, the possible sensors location correspond to the nodes resulting from domain discretization (Fig. 3), but only the points from mould subdomain have been taken into account. Both the basic problem and the sensitivity task have been solved using the explicit scheme of FDM. A priori estimates of mould thermophysical parameters c_{m}, λ_{m} correspond to the values $c_{\mathrm{m}}^0 = 1\,\mathrm{MJ/(m^3K)}$, $\lambda_{\mathrm{m}}^0 = 0.5\,\mathrm{W/(m\,K)}$. The obtained optimal positions of the sensors are marked by A and B in Fig. 8.

The second example concerns the optimal position of three sensors used for simultaneous estimation of casting parameters, in particular Q_{aus} and Q_{eu} (cf. Eq. 7). The geometry of system casting-mould is the same as previously, the possible sensors locations correspond to the FDM nodes and entire domain has been taken into account. Apriori estimates of casting thermophysical parameters Q_{aus}, Q_{eu} correspond to the values $Q_{\mathrm{aus}} = 0$ and $Q_{\mathrm{eu}} = 0$. The obtained optimal positions of the sensors are marked by C, D and E in Fig. 8.

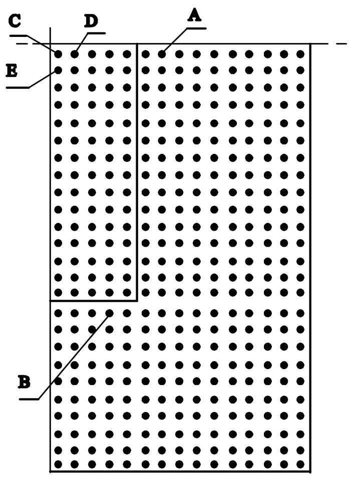

Fig. 8. Optimal sensors position

5. Inverse problem

To solve the inverse problem the additional information concerning the course of process analyzed is necessary. So, let us assume that the values $T_{d\,i}^f$ at the set of points x^i for times t_f are known (cf. Eq. (17)).

Now, the least squares criterion is applied [11–13]

$$S = \frac{1}{MF} \sum_{i=1}^{M} \sum_{j=1}^{F} \left(T_i^f - T_{d\,i}^f \right)^2, \tag{29}$$

where $T_{d\,i}^f$ and $T_i^f = T\left(x^i, t^f\right)$ are the measured and estimated temperatures, respectively. The estimated temperatures are obtained from the solution of direct problem (cf. Section 2) by using the current available estimates for the unknown parameters.

In the case of typical gradient method application [12, 17, 24] the criterion (13) is differentiated with respect to the unknown parameters p_e, $e = 1, 2, \ldots, E$, and next the necessary condition of optimum is used

$$\frac{\partial S}{\partial p_e} = \frac{2}{MF}\sum_{i=1}^{M}\sum_{j=1}^{F}\left(T_i^f - T_{d\,i}^f\right)\left(Z_{i\,e}^f\right)^k = 0, \tag{30}$$

where

$$\left(Z_{i\,e}^f\right)^k = \left.\frac{\partial T_i^f}{\partial p_e}\right|_{p_e = p_e^k} \tag{31}$$

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

Function T_i^f is expanded into a Taylor series about known values of p_l^k; this means

$$T_i^f = \left(T_i^f\right)^k + \sum_{l=1}^{E}\left(Z_{i\,l}^f\right)^k \Delta p_l^k, \tag{32}$$

where

$$\Delta p_l^k = p_l^{k+1} - p_l^k. \tag{33}$$

Putting (32) into (30) one obtains ($e = 1, 2, \ldots, E$)

$$\sum_{i=1}^{M}\sum_{f=1}^{F}\sum_{l=1}^{E}\left(Z_{i\,l}^f\right)^k\left(Z_{i\,e}^f\right)^k \Delta p_l^k = \sum_{i=1}^{M}\sum_{f=1}^{F}\left(T_{d\,i}^f - \left(T_i^f\right)^k\right)\left(Z_{i\,e}^f\right)^k. \tag{34}$$

This system of equations allows to find the values of Δp_e^k and next, on the basis of formula

$$p_e^{k+1} = p_e^k + \Delta p_e^k, \tag{35}$$

the values of p_e^{k+1} for $e = 1, 2, \ldots, E$. The iteration process is stopped when the assumed number of iterations K is achieved.

In Fig. 10 the cooling curves at the control points 1, 2, 3 from casting subdomain (cf. Fig. 9) are shown, while Fig. 11 illustrates the heating curves at the points 4, 5, 6 from the mould subdomain.

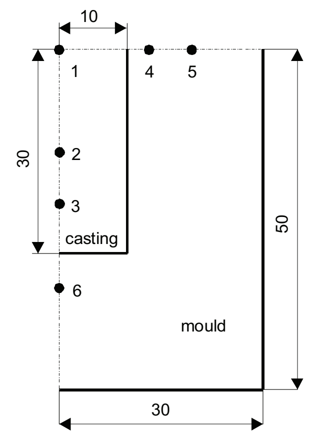

Fig. 9. Position of sensors

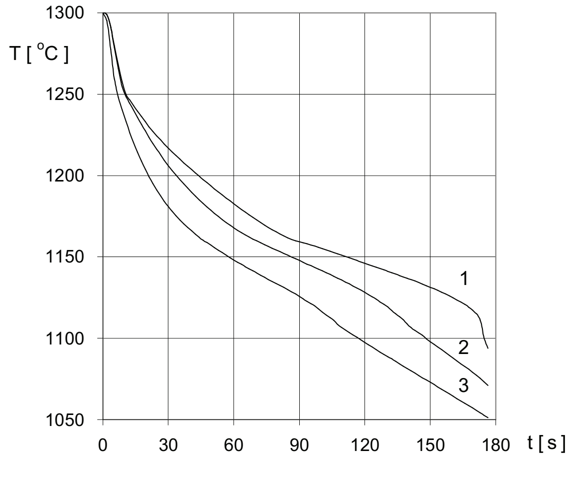

Fig. 10. Cooling curves at the points 1, 2, 3

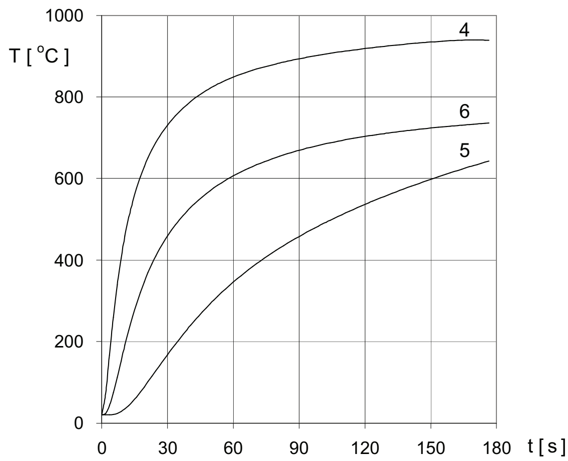

Fig. 11. Heating curves at the points 4, 5, 6

Using cooling (heating) curves presented above, the different inverse problems have been solved [39]. The first solutions have been connected with the identification of a single parameter, among others the estimation of thermal conductivity of mould or thermal conductivity of cast iron. For the assumed initial values λ_{m}^0, λ^0 the iteration process was always convergent and the exact results have been obtained after 5, 6 iterations [39].

The simultaneous identification of two parameters (cast iron and mould thermal conductivities) has been also done. The testing computations showed that for initial values $\lambda^0 \in [5, 45]$, $\lambda_{\mathrm{m}}^0 \in [0.6, 1.9]$ when the all cooling (heating) curves from Figs. 10 and 11 have been taken into account, the iteration process proved to be convergent and the real values of estimated parameters have been obtained after 8–10 iterations [39].

Another example of inverse problem solution was associated with the simultaneous identification of the latent heats Q_{aus}, Q_{eu} connected with the austenite and eutectic phases evolution (cf. Eq. (7)). In this case the initial values constituting a start point for the iteration process have been assumed as $Q_{\mathrm{aus}}^0 = 0$, $Q_{\mathrm{eu}}^0 = 0$. Figure 12 presents the inverse problem solution obtained using the cooling curves at the points 1, 2, 3 (Figs. 9 and 10), while Fig.13 presents the solution using the cooling curves at the optimal points C, D, E (Fig. 8). Comparison of these results confirms that the optimal sensors location assures better estimation of unknown parameters. The iteration process is convergent and the number of iterations is not high.

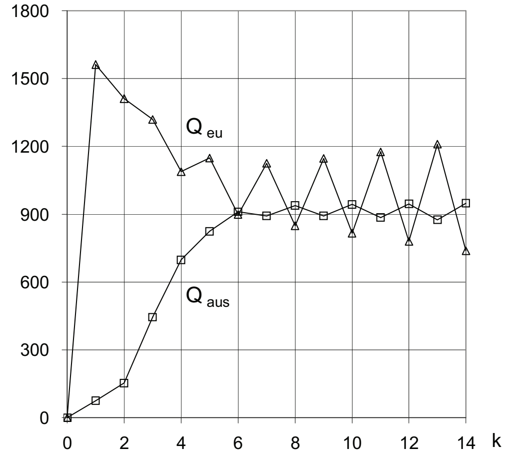

Fig. 12. Identification of Q_{aus} and Q_{eu} (sensors 1, 2, 3 – Fig. 9)

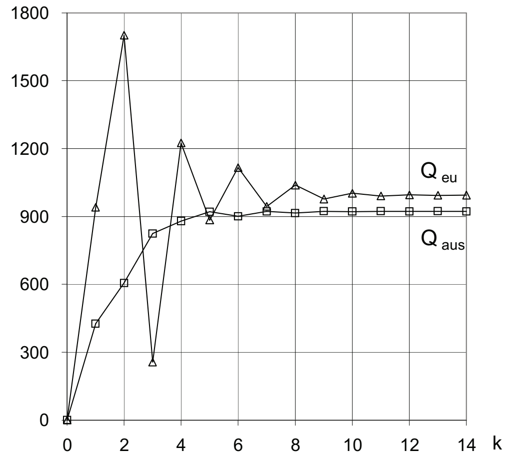

Fig. 13. Identification of Q_{aus} and Q_{eu} (optimal sensors C, D, E – Fig. 8)

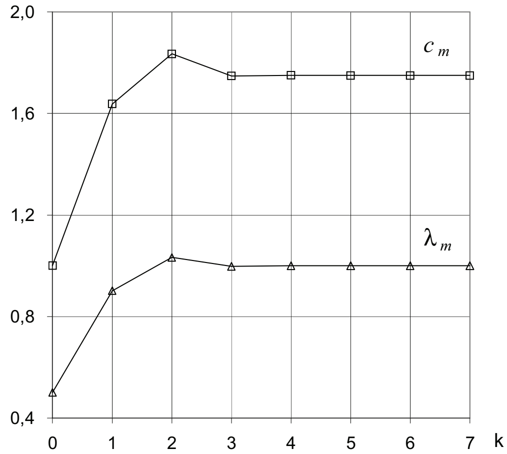

Fig. 14. Inverse problem solution (c_{m}, λ_{m})

The next inverse problem has been connected with the simultaneous identification of mould parameters. This means the thermal conductivity λ_{m} and the volumetric specific heat c_{m}.

This problem has been solved using optimal sensors location (points A and B in Fig. 8) under the assumption that $\lambda_{\mathrm{m}}^0 = 0.5\,\mathrm{W/(m\,K)}$ and $c_{\mathrm{m}}^0 = 1\,\mathrm{MJ/(m^3K)}$. The results of identification are presented in Fig. 14. It is seen that the iteration process is convergent and the number of iterations is very small.

It is possible to identify simultaneously a greater number of parameters [31, 39]. As an example, the estimation of three parameters concerning subdomain casting is presented. On the basis of cooling curves shown in Fig. 10, the simultaneous identification of latent heats Q_{aus}, Q_{eu} and thermal conductivity λ have been done – Fig. 15. In this case the number of iterations is greater and the oscillations appear in the obtained solution, but the final results of identification are still correct.

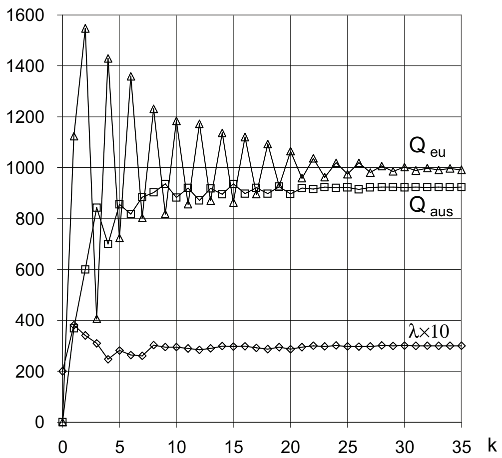

Fig. 15. Identification of Q_{aus}, Q_{eu}, λ

6. Final remarks

In the paper the new possibilities of numerical methods application in the thermal theory of foundry processes are presented. The most valuable results concern the problems of optimum sensors location. Transient and strongly nonlinear task is considered and it constitutes the essential generalization of the algorithms discussed in literature. The simultaneous identification of greater number of thermophysical parameters (both casting and mould are taken into account) was not, up to now, realized. It turned out that this type of inverse problems can be also effectively solved.

In this paper the input data used for the parameters estimation result from the numerical solution of direct problem. The next investigations should concern the application of real input data resulting from the measurements done in the industrial conditions [40].

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