Identification of macro and micro parameters in solidification model

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Abstract. In the paper the thermal processes proceeding in the solidifying metal are analyzed. The basic energy equation determining the course of solidification contains the component (source function) controlling the phase change. This component is proportional to the solidification rate $\partial f_S/\partial t(f_S \in [0, 1])$, is a temporary and local volumetric fraction of solid state. The value of $f_S$ can be found, among others, on the basis of laws determining the nucleation and nuclei growth. This approach leads to the so called micro/macro models (the second generation models). The capacity of internal heat source appearing in the equation concerning the macro scale (solidification and cooling of domain considered) results from the phenomena proceeding in the micro scale (nuclei growth). The function $f_S$ can be defined as a product of nuclei density $N$ and single grain volume $V$ (a linear model of crystallization) and this approach is applied in the paper presented. The problem discussed consists in the simultaneous identification of two parameters determining a course of solidification. In particular it is assumed that nuclei density $N$ (micro scale) and volumetric specific heat of metal (macro scale) are unknown. Formulated in this way inverse problem is solved using the least squares criterion and gradient methods. The additional information which allows to identify the unknown parameters results from knowledge of cooling curves at the selected set of points from solidifying metal domain. On the stage of numerical realization the boundary element method is used. In the final part of the paper the examples of computations are presented.

Key words: micro/macro model of solidification, inverse problems, boundary element method, numerical modelling.

1. Introduction

The thermal processes proceeding in domain of solidifying metal or (more generally) in the system casting-mould are described by the Fourier-Kirchhoff equation, this means a nonlinear parabolic partial differential equation (or the system of such equations) supplemented by the adequate physical, geometrical, boundary and initial conditions. The energy equation for casting domain contains the term describing the capacity of internal heat source (source function) and this term controls the evolution of latent heat connected with the phase change. The solidification models basing on the Fourier-Kirchhoff equation can be divided (according to the classification proposed by Stefanescu [1]) into two groups, namely the macro models and the micro/macro ones. The difference between macro and micro/macro models consists in the way of source function modelling. The typical procedure in the case of macro approach reduces to the assumption that the dependence between a local volumetric fraction of solid state $f_S$ and temperature $T$ is known and then after the mathematical manipulations one obtains the energy equation referring to the whole, conventionally homogeneous, metal domain in which the parameter called a substitute thermal capacity appears (e.g. [2,3]). In the case of micro/macro models (used in this paper) the function $f_S$ is determined on the basis of laws concerning the nucleation and nuclei growth, this means the phenomena proceeding on the micro level (e.g. [4–8]). The direct problems concerning the solidification and cooling processes in the casting-mould system can be solved using the numerical methods and in literature (among others the books and papers quoted previously) one can find the precise information in this scope both for the case of macro and micro/macro modelling.

The inverse problems appearing in the thermal theory of foundry processes consist in the identification of casting-mould internal parameters (e.g. specific heats or thermal conductivities [9,10]), boundary conditions or initial temperatures. In the case of micro/macro models the nuclei density [11], growth coefficient or grains shape coefficient can be also identified. In this paper ‘a mixed task’ is considered. On the basis of cooling curves at selected set of points from metal domain simultaneously the macro and micro/macro internal parameters are determined. As an example the volumetric specific heat of metal (a macro parameter) and the nuclei density (a micro one) are taken into account. The details concerning the mathematical description of the problem, the method of inverse problem solution and the results of computation will be presented in the next chapters.

2. Governing equations

The equation describing the solidification process (only heat conduction is taken into account) can be written in

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the following form
\[
c(T) \frac{\partial T(x,t)}{\partial t} = \nabla [\lambda(T) \nabla T(x,t)] + Q(x,t)
\] (1)
where \( c \) is a volumetric specific heat, \( \lambda \) is a thermal conductivity, \( Q \) is a source term, \( T, x, t \) denote the temperature, geometrical co-ordinates and time. Function \( Q \) is proportional to a solidification rate, this means
\[
Q(x,t) = L \frac{\partial f_s(x,t)}{\partial t}
\] (2)
where \( L \) is a volumetric latent heat, \( f_s \) is a volumetric solid state fraction at the considered point from metal domain. Finally
\[
c(T) \frac{\partial T(x,t)}{\partial t} = \nabla [\lambda(T) \nabla T(x,t)] + L \frac{\partial f_s(x,t)}{\partial t}
\] (3)
On the outer surface of the system the condition in general form
\[
\Phi \left[ T(x,t), \frac{\partial T(x,t)}{\partial n} \right] = 0
\] (4)
is given, where \( \partial / \partial n \) denotes a normal derivative. The initial condition
\[
t = 0 : T(x,0) = T_0
\] (5)
is also known.

The equations above presented constitute (as was mentioned previously) a base of numerical simulation both in the case of macro models of solidification and in the case of micro/macro ones.

The micro/macro model of solidification (the second generation one [4]) basing on the assumption that the kinetics of nucleation and nuclei growth is proportional to the undercooling below the solidification point is considered. So, the driving force of the process is a difference between solidification point \( T_{cr} \) and temporary local temperature – Fig. 1.

\[
\Delta T(x,t) = T_{cr} - T(x,t)
\] (6)

At first, the following function is introduced
\[
\omega(x,t) = N(x,t)V(x,t)
\] (7)
where \( N \) is a grains density \([\text{grains/m}^3]\), \( V \) is a single grain volume. If one considers the spherical grains and \( u = \partial R / \partial t \) is a crystallization rate (\( R \) is a grain radius) then
\[
V(x,t) = \frac{4}{3} \pi \nu N(x,t) \left[ \int_0^t u(x,\tau) \, d\tau \right]^3
\] (8)
In the case of the others types of crystallization (e.g. dendritic growth) the shape coefficient \( \nu < 1 \) can be introduced [6] and then
\[
\omega(x,t) = \frac{4}{3} \pi \nu N(x,t) \left[ \int_0^t u(x,\tau) \, d\tau \right]^3
\] (9)
In the case of so-called linear [5] model the function \( f_s \) is assumed to be equal directly to \( \omega(x,t) \)
\[
f_s(x,t) = N(x,t)V(x,t)
\] (10)
and if \( f_s = 1 \) then the crystallization process stops. The derivative of \( f_s \) with respect to time equals
\[
\frac{\partial f_s(x,t)}{\partial t} = 4\pi \nu \left[ \frac{R(x,t)^3}{3} \frac{\partial N(x,t)}{\partial t} + R(x,t)^2 \frac{\partial R(x,t)}{\partial t} N(x,t) \right]
\] (11)
Assuming the constant number of nuclei (e.g. [8]) we obtain
\[
\frac{\partial f_s(x,t)}{\partial t} = 4\pi \nu N R(x,t)^2 \frac{\partial R(x,t)}{\partial t}
\] (12)
and this case will be below discussed.

In literature the exponential model resulting from the theory proposed by Mehl, Johnson, Avrami and Kolmogoroff (e.g. [4,7]) can be also found. Then
\[
f_s(x,t) = 1 - \exp \left[ -\omega(x,t) \right]
\] (13)
For the small geometrical volumes \( \exp(-\omega) = 1 - \omega \) and then the formulas (10), (13) lead to the same results. In this paper the linear model is considered because the numerical approximation of source function in the energy equation and equations resulting from the sensitivity analysis (see: next chapter) is essentially simpler, while the results are very close.

Additionally it is assumed that the nuclei growth is determined by the formula [7,8]
\[
\frac{\partial R(x,t)}{\partial t} = \mu [T_{cr} - T(x,t)]^2 - \mu \Delta T(x,t)^2
\] (14)
where \( \mu \) is the growth coefficient.
Finally, the local value of source term for $N = \text{const}$ results from the following equation
\[ L \frac{\partial f_S(x,t)}{\partial t} = 4\pi\nu LN\mu \Delta T(x,t)^2 \left[ \int_0^t \mu \Delta T(x,\tau)^2 \, d\tau \right]^2. \] (15)

3. Sensitivity with respect to nuclei density and specific heat

The presented solution of inverse problem bases on the sensitivity coefficients [12]. Because the nuclei density $N$ and volumetric specific heat $c(T) = c = \text{const}$ are identified therefore the sensitivity models concerning these parameters must be constructed (the direct approach is used [12–14]).

Differentiating the energy equation with respect to $N$ one has
\[ c \frac{\partial}{\partial N} \left[ \frac{\partial T(x,t)}{\partial t} \right] = \frac{\partial}{\partial N} \{ \nabla [\lambda(T) \nabla T(x,t)] \}
+ L \frac{\partial}{\partial N} \left[ \frac{\partial f_S(x,t)}{\partial t} \right]. \] (16)

Using the Schwarz theorem and denoting $\partial T/\partial N = U_1$ one obtains
\[ c \frac{\partial U_1(x,t)}{\partial t} = \nabla [\lambda(T) \nabla U_1(x,t)] + Q_U. \] (17)

The source function $Q_U$ in equation (17) equals
\[ Q_U(x,t) = 4\pi\nu L \mu \Delta T(x,t)^2 \]
\[ \times \left[ \int_0^t \mu \Delta T(x,\tau)^2 \, d\tau \right]^2 \left[ \Delta T(x,t) - 2NU_1(x,t) \right] \]
\[ - 16\pi\nu LN\mu \Delta T(x,t)^2 \int_0^t \mu \Delta T(x,\tau)^2 \, d\tau \]
\[ \times \int_0^t \mu \Delta T(x,\tau) U_1(x,\tau) \, d\tau. \] (18)

Denoting
\[ R(x,t) = \int_0^t \mu \Delta T(x,\tau)^2 \, d\tau, \] (19)
\[ R_U(x,t) = \int_0^t \mu \Delta T(x,\tau) U_1(x,\tau) \, d\tau \]

one has
\[ Q_U(x,t) = 4\pi\nu L \mu \Delta T(x,t)^2 R(x,t)^2 \]
\[ \times [\Delta T(x,t) - 2NU_1(x,t)] \]
\[ - 16\pi\nu LN\mu \Delta T(x,t)^2 R(x,t) R_U(x,t). \] (20)

The expression determining source term $Q_U$ is rather complex, but in numerical realization it does not cause the essential difficulties.

Sensitivity equation is supplemented by the initial condition $U_1(x,0) = 0$, and the boundary one in general form
\[ \Phi \left[ U_1(x,t), \frac{\partial U_1(x,t)}{\partial n} \right] = 0. \] (21)

For example, in the case of Robin boundary condition $-\lambda \partial T/\partial n = \alpha(T - T_a)$ ($\alpha$ is a heat transfer coefficient, $T_a$ is an ambient temperature) we have $-\lambda \partial U_1/\partial n = \alpha U_1$.

Sensitivity model concerning the volumetric specific heat requires the differentiation of energy equation and boundary-initial conditions with respect to $c$. So
\[ \frac{\partial T(x,t)}{\partial t} + c \frac{\partial U_2(x,t)}{\partial t} = \nabla [\lambda(T) \nabla U_2(x,t)] + Q_U \] (22)
where $U_2 = \partial T/\partial c$ and
\[ Q_U(x,t) = -8\pi\nu LN\mu \Delta T(x,t) R(x,t) \]
\[ \times [U_2(x,t) R(x,t) + 2\Delta T(x,t) R_U(x,t)] \] (23)
at the same time
\[ R(x,t) = \int_0^t \mu \Delta T(x,\tau)^2 \, d\tau, \] (24)
\[ R_U(x,t) = \int_0^t \mu \Delta T(x,\tau) U_2(x,\tau) \, d\tau. \]

The boundary and initial conditions are the same as previously.

Both the sensitivity model with respect to $N$ and $c$ are strongly coupled with the basic one and the sensitivity problems can be solved under the condition that the basic solution is known.

4. Identification of unknown parameters

If $T_d(x,t)$ is the ‘measured’ (postulated) temperature field in the domain $\Omega$, while $T(x,t)$ is a temperature field found for the assumed values of unknown parameters then the best solution corresponds to the minimum of functional [15,16]
\[ S = \int_0^T \int_\Omega [T(x,t) - T_d(x,t)]^2 \, d\Omega dt \Rightarrow \text{MIN} \] (25)
where $[0,t^F]$ is a time interval considered.

Because, as a rule, the information concerning $T_d$ is given in discrete form (the values of temperature at the set of control points – sensors $x_i$, $i = 1, 2, ..., M$ for times $t^0, t^1, ..., t^F$) therefore the criterion (25) is formulated in the form
\[ S = \sum_{f=0}^F \sum_{i=1}^M [T(x_i,t^f) - T_d(x_i,t^f)]^2 \Rightarrow \text{MIN} \] (26)
or more generally
\[ S = \sum_{f=0}^{F} \sum_{i=1}^{M} \gamma_i \left[ T(x_i,t^f) - T_d(x_i,t^f) \right]^2 \Rightarrow \text{MIN} \] (27)
where \( \gamma_i > 0 \) are the tapering functions.

The necessary condition of functional (26) minimum leads to the equations
\[
\begin{align*}
\frac{\partial S}{\partial N} &= 2 \sum_{i=1}^{M} \sum_{f=1}^{F} \left( T_i^f - T_d^f \right) \frac{\partial T}{\partial N} \bigg|_{\eta = N^k} = 0 \\
\frac{\partial S}{\partial c} &= 2 \sum_{i=1}^{M} \sum_{f=1}^{F} \left( T_i^f - T_d^f \right) \frac{\partial T}{\partial c} \bigg|_{c = c^k} = 0
\end{align*}
\] (28)
where \( T_d^f = T_d(x_i,t^f), T_i^f = T(x_i,t^f) \), \( N^k, c^k \) for \( k = 0 \) are the initial values (start point), while for \( k > 1 \) result from the previous computations. Introducing the sensitivity functions we have
\[
\begin{align*}
\sum_{i=1}^{M} \sum_{f=1}^{F} \left( T_i^f - T_d^f \right) (U_{1i}^k)^2 &= 0 \\
\sum_{i=1}^{M} \sum_{f=1}^{F} \left( T_i^f - T_d^f \right) (U_{2i}^k)^2 &= 0
\end{align*}
\] (29)

Now the function \( T_i^f \) is expanded into Taylor series, namely
\[ T_i^f = (T_i^0)^k + (U_{1i}^k)(N^{k+1} - N^k) + (U_{2i}^k)(c^{k+1} - c^k). \] (30)

Introducing (30) into (29) one obtains
\[
\sum_{i=1}^{M} \sum_{f=1}^{F} \left( U_{1i}^k \right)^2 \sum_{i=1}^{M} \sum_{f=1}^{F} \left( U_{1i}^k \right)^2 + \sum_{i=1}^{M} \sum_{f=1}^{F} \left( U_{2i}^k \right)^2 \sum_{i=1}^{M} \sum_{f=1}^{F} \left( U_{2i}^k \right)^2 \times \left[ N^{k+1} - N^k \right] = \sum_{i=1}^{M} \sum_{f=1}^{F} \left( U_{1i}^k \right)^2 \left( T_{1i}^f - T_i^f \right)^k \sum_{i=1}^{M} \sum_{f=1}^{F} \left( U_{2i}^k \right)^2 \left( T_{2i}^f - T_i^f \right)^k. \] (31)

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 \( c \).

5. Boundary element method

The primary and also the additional problems resulting from the sensitivity analysis have been solved using the 1st scheme of the BEM for transient heat diffusion [17–19]. So, the following Fourier equation will be considered
\[ c \frac{\partial F(x,t)}{\partial t} = \lambda \nabla^2 F(x,t) + Z(x,t) \] (32)
where \( F(x,t) \) denotes the temperature or functions resulting from the sensitivity analysis, while \( Z(x,t) \) is the source function (for primary problem: \( Z(x,t) = Q(x,t) \), for additional problems: \( Z(x,t) = Q_d(x,t) \)). One can see that both \( c \) and \( \lambda \) are assumed to be the constant values. Taking into account the rather small temperature interval in which the process discussed proceeds, such assumption is entirely acceptable. The details concerning the BEM application in the case \( c = c(T) \) and \( \lambda = \lambda(T) \) can be found in [17].

So, at first, the time grid is introduced
\[ 0 = t^0 < t^1 < \ldots < t^{f-1} < t^f < \ldots < t^F < \infty, \] (33)
\[ \Delta t = t^f - t^{f-1}. \]

If the 1st scheme of the BEM is taken into account then the boundary integral equation corresponding to transition \( t^{f-1} \rightarrow t^f \) is of the form
\[
\begin{align*}
B(\xi) F(\xi,t^f) + \frac{1}{c} \int_{t^{f-1}}^{t^f} \int F^*(\xi,x,t^f,t) J(x,t) d\Gamma dt \\
= \frac{1}{c} \int_{t^{f-1}}^{t^f} \int J^*(\xi,x,t^f,t) F(x,t) d\Gamma dt \\
+ \int_{\Omega} F^*(\xi,x,t^f,t^{f-1}) F(x,t^{f-1}) d\Omega \\
+ \frac{1}{c} \int_{t^{f-1}}^{t^f} \int_{\Omega} Z(x,t) F^*(\xi,x,t^f,t) d\Omega dt.
\end{align*}
\] (34)

In Eq. (34) \( F^* \) is the fundamental solution [17–19] and
\[
F^*(\xi,x,t^f,t) = \frac{1}{4\pi a (t^f - t)^{d/2}} \exp \left[ -\frac{r^2}{4a(t^f - t)} \right]
\] (35)
where \( d \) is the dimension of the problem, \( r \) is the distance from the point under consideration \( x \) to the observation point \( \xi \), \( a = \lambda / c \), while
\[
\begin{align*}
J^*(\xi,x,t^f,t) &= -\lambda \frac{\partial F^*(\xi,x,t^f,t)}{\partial n}, \\
J(x,t) &= -\lambda \frac{\partial F(x,t)}{\partial n},
\end{align*}
\] (36)
and \( B(\xi) \) is the coefficient from the interval \((0,1)\).

We use the constant elements with respect to time [17,18] and then the boundary integral Eq. (34) takes a form
\[
B(\xi) F(\xi,t^f) + \int_{\Gamma} J(x,t^f) g(\xi,x) d\Gamma \\
= \int_{\Gamma} F(x,t^f) h(\xi,x) d\Gamma + \int_{\Omega} J^*(\xi,x,t^f,t^{f-1}) \\
\times F(x,t^{f-1}) d\Omega + \int_{\Omega} Z(x,t^{f-1}) g(\xi,x) d\Omega
\] (37)
where
\[ h(\xi,x) = \frac{1}{c} \int_{t^{f-1}}^{t^f} J^*(\xi,x,t^f,t) dt \] (38)
and
\[
g(\xi, x) = \frac{1}{c} \int_{t^{f}}^{t} F^{*}(\xi, x, t^{f}, t) dt. \tag{39}
\]

In numerical realization the following discrete form of the boundary integral Eq. (37) is considered
\[
\sum_{j=1}^{N} G_{ij} J_{j}^{f} = \sum_{j=1}^{N} H_{ij} F_{j}^{f} + \sum_{l=1}^{L} P_{il} F_{l}^{f-1} + \sum_{l=1}^{L} W_{il} Z_{l}^{f-1} \tag{40}
\]
where
\[
G_{ij} = \int g(\xi^{i}, x) d\Gamma_{j}, H_{ij} = \begin{cases} \int h(\xi_{j}, x) d\Gamma_{j}, i \neq j \\ -0.5, \quad i = j \end{cases}
\tag{41}
\]
and
\[
P_{il} = \int_{\Omega_{l}} F^{*}(\xi^{i}, x, t^{f}, t^{f-1}) d\Omega_{l}, \quad W_{il} = \int_{\Omega_{l}} g(\xi^{i}, x) d\Omega_{l}. \tag{42}
\]

The system of Eq. (40) can be written in the matrix form, namely
\[
G \cdot J^{f} = H \cdot F^{f} + P \cdot F^{f-1} + W \cdot Z^{f-1}. \tag{43}
\]

After determining the ‘missing’ boundary values of \( F \) and \( J \), the values of function \( F \) at the internal points \( \xi^{i} \) for time \( t^{f} \) are calculated using the formula \((i = N + 1, ..., N + L)\):
\[
F_{i}^{f} = \sum_{j=1}^{N} H_{ij} F_{j}^{f} - \sum_{j=1}^{N} G_{ij} J_{j}^{f} + \sum_{l=1}^{L} P_{il} F_{l}^{f-1} + \sum_{l=1}^{L} W_{il} Z_{l}^{f-1}. \tag{44}
\]

6. Example of computations

The algorithm above presented can be used both in the case of 1D problem and 2D or 3D ones. It is only the problem of adequate computer program construction. Below the solution concerning the aluminium plate \((G = 3 \text{ cm} - 1 \text{D task})\) will be shown. The influence of mould is taken into account by the Robin condition for \( x = -1.5 \) and \( x = 1.5 \) (heat transfer coefficient \( \alpha = 250 \text{ W/(m}^{2}\text{K})\)). Nuclei density \( N = 10^{10} \), volumetric specific heat \( c = 2.875 \text{ MJ/(m}^{3}\text{K})\), the other parameters of material [2]: \( \lambda = 150 \text{ W/(mK)}\), \( L = 975 \text{ MJ/m}^{3}\), \( \mu = 3 \cdot 10^{-6} \text{ m/(sK}^{2})\), solidification point \( T_{cr} = 660^\circ\text{C}\), pouring temperature \( T_{0} = 670^\circ\text{C}\). The cooling curves corresponding to the basic solution are shown in Fig. 2. The inverse problem has been solved under the assumption that the cooling curves are known, at the same time the different initial values of estimated parameters have been taken into account, for example \( N^{0} = 10^{8}, c^{0} = 2 \) (variant 1) and \( N^{0} = 10^{8}, c^{0} = 3.5 \) (variant 2). In Figs. 3, 4 the results of identification this means the values of \( N^{k}/N_{d} \) and \( c^{k}/c_{d} \) \((N_{d} = 10^{10}, c_{d} = 2.875\) denote the real values of parameters) for successive iterations are shown. It is visible that the iteration process is convergent and real values of identified parameters are obtained after a few iterations. The testing computations show that iteration process is convergent even for initial value of nuclei \( N^{0} = 1 \) and from numerical point of view it is very important information. It appears that the values \( N^{0} = 1 \) and \( c^{0} \in [1, 6] \) assure the convergence of simultaneous identification of the parameters \( N \) and \( c \). Figs. 5 and 6 illustrate the solutions.
of inverse problem for $N^0 = 1, c^0 = 6$ (variant 3) and $N^0 = 1, c^0 = 1$ (variant 4).

In the next version of computations in the place of $T_d(x_i, t_f)$ the disturbed data (in relation to the basic solution) have been introduced. The ‘exact’ solution has been transformed randomly using the procedure described in [20]. In Fig. 7 the example of cooling curves obtained in this way is presented. The results of identification corresponding to successive iterations are shown in Fig. 8 ($N^0 = 1, c^0 = 1$). One can see that the iterative process is convergent and the final values of $N$ and $c$ are sufficiently exact.

7. Conclusions

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
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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). It should be pointed out that the model of solidification presented here concerns a small superheating of metal because only heat conduction is considered. The simplification consisting in ‘rejection’ of mould subdomain and approximation of the mould influence by the Robin condition on the external surface of casting is not necessary (e.g. [8]). It was introduced here in order to simplify the theoretical considerations connected with the main subject of this paper.

Fig. 8. Simultaneous identification of \( N \) and \( c \) – disturbed data \( (1 - N^k/N_d, \ 2 - c^k/c_d) \)

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