Application of identification methods in solidification process modelling

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Abstract

In the paper the identification problems connected with the estimation of cast iron and mould thermophysical parameters are discussed. The additional information necessary to solve the problem results from a 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 on the present stage of research the numerical solution of direct problem plays a role of measured temperatures. The identification algorithm basing on the gradient methods is used to estimate the parameters of casting–mould system (a case of simultaneous estimation of bigger number of parameters is also considered). On the stage of numerical realization the FDM is used (2D task). In the final part of the paper the examples of computations are shown.

Keywords: Application of Information Technology to the Foundry Industry; Solidification Process; Numerical Techniques; 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 the different variants of input data concerning the details of casting-mould geometry, initial temperatures, properties of mould sub-domain etc., one can determine the variant of technology assuring the good quality of final product. The base of numerical model construction results from the assumed mathematical description of the thermal processes proceeding in the system considered [1, 2, 3]. This model, as a rule, 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 typical model of casting solidification belongs to a group of so-called direct problems (the physical, boundary and initial parameters appearing in the mathematical description are known). The other task appears in the case when the part of process parameters is unknown, then the inverse problem must be solved [4, 5, 6, 7, 8]. The solution of inverse problem (identification problem) can be found under the condition that one disposes the additional information concerning the course of the process. This information can be obtained by the measurements of cooling (heating) curves at the points selected from the casting–mould domain. On a stage of identification algorithm construction the real measurements are substituted by a direct problem solution (or this solution disturbed in a random way). In literature one can find the different methods of identification problem solution, here the gradient method basing on the least squares criterion and sensitivity coefficients has been used [9, 10]. In the simplest version of computations only single parameters have been identified, more complex tasks concerned the simultaneous identification of the bigger number of unknown parameters. On a stage of numerical modelling the finite difference method for non-linear parabolic equation has been applied. In the final part of the paper the examples of parameters estimation are shown.
2. Direct problem

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

\[ x \in \Omega : \quad c(T) \frac{\partial T(x, t)}{\partial t} = \nabla \cdot (\lambda(T) \nabla T(x, t)) + L \frac{df_s(x, t)}{dt} \]  \hspace{1cm} (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 the casting domain, \( T, x, t \) denote the temperature, geometrical co-ordinates and time.

If one assumes the constant value of thermal conductivity \( \lambda \) of the casting material then the equation (1) can be expressed as follows

\[ x \in \Omega : \quad c(T) \frac{\partial T(x, t)}{\partial t} = \lambda \nabla^2 T(x, t) \]  \hspace{1cm} (2)

In the case of typical macro model (the one domain approach [1, 4, 10]), we assume knowledge of temperature-dependent function \( f_s(T) \) in the mushy zone \( T \in [T_s, T_L] \) sub-domain and then

\[ \frac{\partial f_s(x, t)}{\partial t} = \frac{d f_s(T)}{dT} \frac{\partial T(x, t)}{\partial t} \]  \hspace{1cm} (3)

So, the equation (2) takes the form

\[ x \in \Omega : \quad C(T) \frac{\partial T(x, t)}{\partial t} = \lambda \nabla^2 T(x, t) \] \hspace{1cm} (4)

where

\[ C(T) = c(T) - L \frac{df_s(T)}{dT} \]  \hspace{1cm} (5)

is called a substitute thermal capacity [1, 7, 10].

It is self-evident that for molten metal and solidified part of casting \( f_s = 0, f_s = 1 \) and then \( df_s/dT = 0 \). Summing up, the equation (4) describes the thermal processes in the whole, conventionally homogeneous, casting domain. The substitute thermal capacity can be written in the form

\[ C(T) = \begin{cases} c_L, & T > T_L \\ c_s - L \frac{df_s(T)}{dT}, & T_s < T \leq T_L \\ c_s, & T \leq T_s \end{cases} \] \hspace{1cm} (6)

where \( T_L, T_s \) correspond to the liquidus and solidus temperatures, respectively, \( c_L, c_s, c_p = 0.5(c_L + c_s) \) are the constant volumetric specific heats of molten metal, solid state and mushy zone sub-domain.

In the case of cast iron solidification the following approximation of substitute thermal capacity can be taken into account (Figure 1) [11]

\[
C(T) = \begin{cases} c_L, & T > T_L \\ \frac{c_L + c_s}{2}, & T_s < T \leq T_L \\ \frac{c_s}{2}, & T \leq T_s \end{cases}
\] \hspace{1cm} (7)

where \( T_e \) is the temperature corresponding to the beginning of eutectic crystallization, \( Q_{am}, Q_{as} \) are the latent heats connected with the austenite and eutectic phases evolution.

\[ T > T_L \]
\[ \frac{c_L + c_s}{2}, \quad T_s < T \leq T_L \]
\[ \frac{c_s}{2}, \quad T \leq T_s \]

Fig. 1. Substitute thermal capacity of cast iron

The considered equation is supplemented by the equation concerning a mould sub-domain

\[ x \in \Omega_m : \quad c_m \frac{\partial T_m(x, t)}{\partial t} = \lambda_m \nabla^2 T_m(x, t) \] \hspace{1cm} (8)

where \( c_m \) is the mould volumetric specific heat, \( \lambda_m \) is the mould thermal conductivity.

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

\[ x \in \Gamma_c : \quad -\lambda_m \nabla T_m(x, t) = -\lambda_m \nabla T_m(x, t) \]
\[ T(x, t) = T_m(x, t) \] \hspace{1cm} (9)

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

\[ x \in \Gamma_s : \quad -\lambda_a \nabla T_m(x, t) = \alpha \left[ T_m(x, t) - T_a \right] \] \hspace{1cm} (10)

is given (\( \alpha \) is the heat transfer coefficient, \( T_a \) is the ambient temperature).

For time \( t = 0 \) the initial condition

\[ t = 0 : \quad T(x, 0) = T_0(x), \quad T_m(x, 0) = T_{m0}(x) \] \hspace{1cm} (11)

is also known.
3. Inverse problem

If the parameters appearing in governing equations are known then the direct problem is analyzed, while if part of them is unknown then the inverse problem should be considered.

The unknown parameters will be denoted by \( p_e, e = 1, 2, ..., E \). For example, if the thermophysical parameters of mould will be identified, then \( p_1 = \lambda_m \) corresponds to the thermal conductivity of mould, \( p_2 = c_m \) corresponds to the mould volumetric specific heat and \( E = 2 \). If it is assumed that the course of substitute thermal capacity is unknown (c.f. equation (7)) and the parameters \( c_L, c_S, Q_{in}, Q_{out} \) should be identified then \( p_1 = c_L, p_2 = c_S, p_3 = Q_{in}, p_4 = Q_{out} \) and \( E = 4 \).

To solve the inverse problem the additional information concerning the process analyzed is necessary. So, it is assumed that the values \( T_{d_i} \) at the set of points \( x_i \) (sensors) selected from the casting-mould domain for times \( t' \) are known.

\[
T_{d_i} = T_j(x_i, t'), \quad i = 1, 2, ..., M, \quad f = 1, 2, ..., F
\]  

(12)

The least squares criterion is applied

\[
S = \frac{1}{M F} \sum_{i=1}^{M} \sum_{f=1}^{F} (T_{d_i} - T_j)^2
\]

(13)

where \( T_j \) (cf equation (12)) and \( T_j = T(x_j, t') \) are the measured and estimated temperatures, respectively. The estimated temperatures are obtained from the solution of the direct problem (cf chapter 1) by using the current available estimate for the unknown parameters.

In the case of typical gradient method application \([9, 13]\) the criterion (13) is differentiated with respect to the unknown parameters \( p_e, e = 1, 2, ..., E \) and next the necessary condition of optimum is used

\[
\frac{\partial S}{\partial p_e} = \frac{2}{M F} \sum_{i=1}^{M} \sum_{f=1}^{F} (T_{d_i} - T_j) (Z_{j_i})^e = 0
\]

(14)

where

\[
(Z_{j_i})^e = \frac{\partial T_j}{\partial p_e} |_{p_e = p_e^*}
\]

(15)

are the sensitivity coefficients, \( k \) is the number of iteration, \( p_e^0 \) are the arbitrary assumed values of \( p_e \), while \( p_e^k \) for \( k > 0 \) result from the previous iteration.

Function \( T_j \) is expanded in a Taylor series about known values of \( p_e^0 \), this means

\[
T_j = (T_j)^0 + \sum_{i=1}^{E} (Z_{j_i})^e \Delta p_i^k
\]

(16)

where

\[
\Delta p_i^k = p_i^{k+1} - p_i^k
\]

(17)

Putting (16) into (14) one obtains (e = 1, 2, ..., E)

\[
\sum_{i=1}^{M} \sum_{j=1}^{F} (Z_{j_i})^e (Z_{j_i})^e \Delta p_i^k = \sum_{i=1}^{M} \sum_{j=1}^{F} [T_{d_i} - (T_j)^0] (Z_{j_i})^e
\]

(18)

The system of equations (18) can be written in the matrix form

\[
(Z)^T Z \Delta p^k = (Z)^T (T_d - T^0)
\]

(19)

where

\[
Z = \begin{bmatrix}
(Z_{j_1})^e & \ldots & (Z_{j_1})^e \\
\vdots & \ddots & \vdots \\
(Z_{j_M})^e & \ldots & (Z_{j_M})^e
\end{bmatrix}
\]

(20)

and

\[
T_d = \begin{bmatrix}
(T_{d_1})^0 \\
\vdots \\
(T_{d_M})^0
\end{bmatrix}, \quad T^0 = \begin{bmatrix}
(T_j)^0 \\
\vdots \\
(T_j)^0
\end{bmatrix}
\]

(21)

while

\[
\Delta p^k = \begin{bmatrix}
p_1^{k+1} - p_1^k \\
p_2^{k+1} - p_2^k \\
\vdots \\
pi^{k+1} - pi^k \\
p_{E}^{k+1} - p_{E}^k
\end{bmatrix}
\]

(22)
This system of equations allows to find the values of $\Delta p_e^k$ and next on the basis of formula

$$p_e^{e+1} = p_e^k + \Delta p_e^k$$

(23)

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

4. Sensitivity functions

To determine the sensitivity coefficients (15) the governing equations (4), (8) – (11) are differentiated with respect to $p_e$ [14, 15, 16]. So, the following additional problems should be solved

$$x \in \Omega : \frac{\partial C(T)}{\partial p_e} \frac{\partial T(x, t)}{\partial t} + C(T) \frac{\partial}{\partial p_e} \left( \frac{\partial T(x, t)}{\partial t} \right) =$$

$$= \lambda \frac{\partial}{\partial p_e} \left[ \nabla^2 T(x, t) \right]$$

$$x \in \Omega_m : c_n \frac{\partial}{\partial p_e} \left( \frac{\partial T_m(x, t)}{\partial t} \right) = \lambda_m \frac{\partial}{\partial p_e} \left[ \nabla^2 T_m(x, t) \right]$$

$$x \in \Gamma_r : \left[ -\lambda_n \nabla T_m(x, t) = \lambda_m \nabla \frac{\partial T_m(x, t)}{\partial p_e} \right]$$

$$x \in \Gamma_0 : -\lambda_m \nabla T_m(x, t) = 0$$

$$t = 0 : \frac{\partial T(x, 0)}{\partial p_e} = 0 , \frac{\partial T_m(x, 0)}{\partial p_e} = 0$$

or

$$x \in \Omega : C(T) \frac{\partial Z_e(x, t)}{\partial t} = \lambda \nabla^2 Z_e(x, t) - \frac{\partial C(T)}{\partial p_e} \frac{\partial T(x, t)}{\partial t}$$

$$x \in \Omega_m : c_n \frac{\partial Z_m(x, t)}{\partial t} = \lambda_m \nabla^2 Z_m(x, t)$$

$$x \in \Gamma_r : \left[ -\lambda_n \nabla Z_m(x, t) = \lambda_m \nabla Z_m(x, t) \right]$$

$$x \in \Gamma_0 : -\lambda_m \nabla Z_m(x, t) = 0$$

$$t = 0 : Z_e(x, 0) = 0 , Z_m(x, 0) = 0$$

where

$$Z_e(x, t) = \frac{\partial T(x, t)}{\partial p_e}, \quad Z_m(x, t) = \frac{\partial T_m(x, t)}{\partial p_e}$$

(25)

and $e = 1, 2, \ldots, E$.

The basic problem for the assumed values of $p_e$ and the additional ones connected with the sensitivity functions $Z_e$ computations have been solved using the explicit scheme of finite difference method [1].

5. Results of computations

The casting-mould system shown in Figure 2 has been considered. At first, the direct problem has been solved. The following input data have been introduced: $\lambda = 30$ [W/(mK)], $\lambda_m = 1$ [W/(mK)], $c_L = 5.88$ [MJ/(m$^3$K)], $c_S = 5.4$ [MJ/(m$^3$K)], $Q_{\text{ext}} = 923$ [MJ/m$^3$], $Q_{\text{in}} = 994$ [MJ/m$^3$], $c_m = 1.75$ [MJ/(m$^3$K)], pouring temperature $T_0 = 1300^\circ$C, liquidus temperature $T_L = 1250^\circ$C, border temperature $T_E = 1160^\circ$C, solidus temperature $T_S = 1110^\circ$C, initial mould temperature $T_{m0} = 20^\circ$C.

The direct problem has been solved using the explicit scheme of FDM [1]. The regular mesh created by 25x15 nodes with constant step $h = 0.002$ [m] has been introduced, time step $\Delta t = 0.1$ [s].

In Figures 3 and 4 temperature distribution in casting and mould for times 90 and 180 s is presented. In Figure 5 the cooling curves at the control points 1, 2, 3 from casting sub-domain (c.f. Figure 2) are shown, while Figure 6 illustrates the heating curves at the points 4, 5, 6 from mould sub-domain.

Using these cooling (heating) curves the several inverse problems have been solved. The first group concerned the identification of single parameter, this means the estimation of constant thermal conductivity of mould (Figures 7, 8) and constant thermal conductivity of cast iron (Figures 9, 10). For the assumed initial values $\lambda_m^0, \lambda_e^0$ of these parameters the iteration process was convergent and the exact results of identification have been obtained after 5, 6 iterations.

Next, the simultaneous identification of cast iron and mould thermal conductivities has been done. The testing computations showed that for initial values $\lambda_m^0 \in [5, 45], \lambda_e^0 \in [0.6, 1.9]$ and the all cooling (heating) curves application (Figures 5, 6) the iteration process was convergent and the real values of estimated parameters have been obtained after 8–10 iterations.
Fig. 3. Temperature distribution in casting sub-domain

Fig. 4. Temperature distribution in mould sub-domain

Fig. 5. Cooling curves at the points 1, 2, 3

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

Fig. 7. Identification of $\lambda_m$ on the basis of curves 4, 5, 6

Fig. 8. Identification of $\lambda_m$ on the basis of curves 1, 2, 3
Figures 11, 12 illustrate the courses of sensitivity functions $\partial T/\partial \lambda$ (Figure 11) and $\partial T/\partial \lambda_{m}$ (Figure 12) at the points 4, 5, 6 obtained for the real values of $\lambda$ and $\lambda_{m}$.

In Figures 13, 14, 15 the results of identification for initial values $\lambda^{0} = 5, \lambda_{m}^{0} = 0.5$ (variant 1); $\lambda^{0} = 50, \lambda_{m}^{0} = 1.9$ (variant 2) and $\lambda^{0} = 5, \lambda_{m}^{0} = 2.3$ (variant 3) are shown. The results are presented in the form $\lambda/\lambda_{r}$, $\lambda_{m}/\lambda_{r}$ where $\lambda_{r} = 30$ denotes the real value of cast iron thermal conductivity and $k$ is the number of iteration.

Next example of inverse problem solution was associated with the simultaneous identification of the latent heats $Q_{ewr}$, $Q_{es}$ connected with the austenite and eutectic phases evolution (c.f. equation (7)). In this case the 'natural' initial values using in the iteration process were $Q_{ewr}^{0} = 0$, $Q_{es}^{0} = 0$. Here, only one sensor (node 1 marked in Figure 2) has been taken into account. In Figures 16, 17 the courses of sensitivity functions $\partial T/\partial Q_{ew}$ and $\partial T/\partial Q_{es}$ at the point 1 for the iterations $k = 0, 1, 2, 3, 4$ are shown. Figure 18 illustrates the results of identification.

Fig. 9. Identification of $\lambda$ on the basis of curves 1, 2, 3

Fig. 10. Identification of $\lambda$ on the basis of curves 4, 5, 6

Fig. 11. Courses of sensitivity function $\partial T/\partial \lambda$ at the points 4, 5, 6

Fig. 12. Courses of sensitivity function $\partial T/\partial \lambda_{m}$ at the points 4, 5, 6

Fig. 13. Identification of $\lambda$ and $\lambda_{m}$ – variant 1
Fig. 14. Identification of $\lambda$ and $\lambda_m$ – variant 2

Fig. 15. Identification of $\lambda$ and $\lambda_m$ – variant 3

Fig. 16. Courses of sensitivity function $\partial T/\partial Q_{\text{aux}}$

Fig. 17. Courses of sensitivity function $\partial T/\partial Q_{\text{ref}}$

Fig. 18. Identification of $Q_{\text{aux}}$ and $Q_{\text{ref}}$

Fig. 19. Identification of $Q_{\text{aux}}, Q_{\text{ref}}, \lambda$
It is possible to identify simultaneously the greater number of parameters. As an example, the estimation of three parameters concerning casting sub-domain is presented. On the basis of cooling curves shown in Figure 3, the simultaneous identification of latent heats \( Q_{\text{eav}}, Q_{\text{ew}} \) and thermal conductivity \( \lambda \) has been done – Figure 19. In this case the number of iterations is bigger and the oscillations in the solution obtained appear, but the final results of identification are still correct.

6. Conclusions

The testing computations show that the identification of single parameter is very simple. The information concerning only one cooling (heating) curve is quite sufficient. The iteration process is quickly convergent even when the start point is assumed far away in relation to the real value. It is also possible to obtain a good estimation of the bigger number of parameters, but the number of iterations is visible bigger. The problem of initial values assumption is also essential because it determines the number of iterations assuring the identification of real values. The process of computations can be also divergent. In such a situation one can apply the improved gradient methods (e.g. the Levenberg–Marquardt algorithm). The next investigations will concern the application of real input data resulting from the measurements done during the course of technological process.

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References


Zastosowanie metod identyfikacji w modelowaniu procesu krzepnięcia

Streszczenie

W pracy przedstawiono problemy identyfikacji związane z estymacją parametrów odlewu żelaznego i masy formierskiej. Dodatkową informacją niezbędną do rozwiązywania tego typu zadań jest znajomość krzywych stężeń (nagrzewania) w zbiorze punktów odlewu/formy. Krzywe stężeń (nagrzewania) można otrzymać na podstawie pomiarów wykonanych w rzeczywistych warunkach przebiegu procesu. Na obecnym etapie badań krzywe te uzyskiwano poprzez rozwiązanie zadania bezpośredniego dla zadanego wpływu parametrów procesu. Algorytmy identyfikacji bazujące na metodach gradientowych zastosowano do estymacji parametrów występujących w układzie odlew-forma. W końcowej części artykułu pokazano przykłady obliczeń.

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