Gradient method of cast iron latent heat identification

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Abstract

In the paper the cast iron latent heat in the form of three components corresponding to solidification of austenite and eutectic phases is identified. The basic information concerning the form of adequate functions approximation has been taken on the basis of cooling curve and temperature derivative courses found by means of the TDA technique. On the stage of inverse problem solution the gradient method has been used. The numerical computations have been done using the finite difference method. In the final part of the paper the example of latent heat identification is shown.

Keywords: Application of information technology to the foundry industry, Solidification process, Numerical techniques, Inverse problems, Gradient methods, Identification of latent heat

1. Introduction

The inverse problems constitute a very effective tool for the analysis of thermal processes proceeding in the system casting-mould-environment. In this paper the parametric inverse problem is discussed, this means the latent heats connected with the cast iron solidification are identified. The values of these parameters determine the course of substitute thermal capacity of metal. The substitute thermal capacity constitutes a very essential parameter appearing in the governing equation determining a casting solidification, in particular when the one domain approach is applied \cite{1, 2, 3}. To identify the latent heats corresponding to austenite and eutectic phases the gradient methods have been used \cite{4, 5, 6, 7, 8}. Additionally, knowledge of cooling (heating) curves at the points selected from casting (mould) domain is necessary to solve the problem considered and a such information (in this paper) results from the numerical solution of direct problem for real values of cast iron parameters.

2. Cast iron substitute thermal capacity

To determine the course of substitute thermal capacity of cast iron the experimental researches have been realized. The heat cast of hypo-eutectic grey cast iron of Z200-Z250 class has been prepared. The charge material has been choosen according to the rules concerning the smelting of cast iron in the induction furnace. In the central part of the sampling casting the thermocouple PtRh-Pt has been installed. The thermocouple has been connected to the registering apparatus. The thermal and derivative analysis (TDA) has been done in order to determine the characteristic temperatures associated with the change transition. So, the heat processes proceeding in the solidifying metal connected with the latent heat emission of successive phases have been registered taking into...
account the cooling curve \( T_d(t) = T(x, t) \) and its time derivative \( \partial T_d(t)/\partial t \). Using the diagrams of the thermal and derivative analysis the values of temperature-dependent latent heat have been registered [9] (Fig. 1).

Next, the substitute thermal capacity distribution for mushy zone containing the information about the austenite and eutectic phases has been described – Fig. 2. Of course, the physical condition in the form

\[
\int_{t_s}^{T_e} C(T)dT = c_p \left( T_L - T_s \right) + Q
\]

must be fulfilled. In equation (1) \( Q = Q_{\text{aus}} + Q_{\text{eu}} \) is the cast iron latent heat, \( Q_{\text{aus}} = Q_{\text{aus1}} + Q_{\text{aus2}} \). \( Q_{\text{eu}} \) are the latent heats connected with the austenite and eutectic phases evolution.

![Fig. 1. Distribution of cast iron latent heat](image)

![Fig. 2. Substitute thermal capacity of cast iron](image)

So, in the case of cast iron solidification the following approximation of substitute thermal capacity can be taken into account (Fig. 2)

\[
C(T) = \begin{cases} 
  c_L, & T \geq T_L \\
  a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4, & T_L \leq T < T_L \\
  c_{\text{de}}, & T_E \leq T < T_A \\
  b_1 + b_2 T + b_3 T^2 + b_4 T^3 + b_5 T^4, & T_A \leq T < T_E \\
  c_S, & T < T_A 
\end{cases} 
\]

where \( T_i, T_0, T_E, T_S \) correspond to the border temperatures, \( a_k, b_k \), \( k = 1, 2, 3, 4, 5 \) are the coefficients and

\[
c_{\text{de}} = c_p + \frac{Q_{\text{eu1}}}{T_A - T_E} 
\]

where \( c_p = 0.5(c_L + c_S) \).

The coefficients \( a_k, b_k \) have been found on the basis of conditions assuring the continuity of \( C^1 \) class and physical correctness of approximation, namely

\[
\begin{align*}
C(T_L) & = c_L \\
C(T_A) & = c_{\text{de}} \\
\left. \frac{dC(T)}{dT} \right|_{T=T_L} & = 0 \\
\left. \frac{dC(T)}{dT} \right|_{T=T_A} & = 0 \\
\int_{t_s}^{T_e} C(T)dT & = c_p \left( T_L - T_s \right) + Q_{\text{eu}}
\end{align*}
\]

After the mathematical manipulations one has

\[
a_1 = \frac{c_{\text{de}}T_L - c_L T_A}{T_L - T_A} + \frac{(c_L - c_{\text{de}})T_A(T_L + T_A)}{(T_L - T_A)^3} + \\
\frac{30T_L^2T_A^2Q_{\text{eu1}}}{(T_L - T_A)^3} \\
a_2 = -\frac{6(c_L - c_{\text{de}})T_A T_L}{(T_L - T_A)^4} - \frac{60T_A T_L (T_L + T_A)Q_{\text{eu1}}}{(T_L - T_A)^3} \\
a_3 = \frac{3(c_L - c_{\text{de}})(T_L + T_A)}{(T_L - T_A)^4} + \frac{30T_L^2 + 47T_A T_L + T_A^2}{(T_L - T_A)}Q_{\text{eu1}} \\
a_4 = -\frac{2(c_L - c_{\text{de}})}{(T_L - T_A)^4} - \frac{60(T_L + T_A)Q_{\text{eu1}}}{(T_L - T_A)^3} \\
a_5 = \frac{30Q_{\text{eu1}}}{(T_L - T_A)^3}
\]
and

\[
b_1 = \frac{c_{al} T_x - c_{al} T_s}{T_x - T_s} + \frac{(c_{al} - c_s) T_x T_s (T_x + T_s)}{(T_x - T_s)^3} + \frac{30 T_x^2 T_s^2 Q_m}{(T_x - T_s)^3} + \frac{30 T_x^2 T_s^2 Q_m}{(T_x - T_s)^3} + \frac{60 T_x T_s (T_x + T_s) Q_m}{(T_x - T_s)^3} + \frac{3 (c_{al} - c_s) (T_x + T_s)}{(T_x - T_s)^3} + \frac{30 (T_x^2 + 4 T_s T_s + T_s^2) Q_m}{(T_x - T_s)^3} \]
\]

where \( T_x \) and \( T_s \) denote the temperature of the casting and the mould, respectively.

3. Governing equations

The energy equation describing the casting solidification has the following form

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

where \( C(T) \) is the substitute thermal capacity of cast iron (c.f. equation (2)), \( \lambda \) is the thermal conductivity, \( T, x, t \) denote the temperature, geometrical co-ordinates and time.

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

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

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

\[
x \in \Gamma_c : \quad -\lambda_n \mathbf{n} \cdot \nabla T(x, t) = -\lambda_m \mathbf{n} \cdot \nabla T_m(x, t) \quad (10)
\]

can be accepted.

On the external surface of the system the Robin condition

\[
x \in \Gamma_0 : \quad -\lambda_m \mathbf{n} \cdot \nabla T_m(x, t) = \alpha[T(x, t) - T_s] \quad (11)
\]

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

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

\[
t = 0 : \quad T(x, 0) = T_0(x) , \quad T_m(x, 0) = T_{m0}(x) \quad (12)
\]

is also known.

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 \([4, 6, 7, 8]\). In the paper the cast iron latent heats \( Q_{aus1}, Q_{aus2} \) and \( Q_{eu} \) are identified. To solve the inverse problem the sensitivity coefficients should be determined \([11, 12]\). So, the additional boundary initial problems resulting from the differentiation of basic equations with respect to the unknown parameters must be formulated.

4. Sensitivity coefficients

To determine the sensitivity coefficients the governing equations (8) – (12) are differentiated with respect to \( p_1 = Q_{aus1}, p_2 = Q_{aus2} \) and \( p_3 = Q_{eu} \). So, the following additional problems should be solved

\[
x \in \Omega : \quad \frac{\partial C(T)}{\partial p}. \frac{\partial T(x, t)}{\partial t} + C(T) \frac{\partial}{\partial p} \left[ \frac{\partial T(x, t)}{\partial t} \right] = \lambda \frac{\partial}{\partial p} \left[ \nabla^2 T(x, t) \right] \quad (13)
\]

or

\[
x \in \Omega_m : \quad c_m \frac{\partial}{\partial p} \left[ \frac{\partial T_m(x, t)}{\partial t} \right] = \lambda_m \frac{\partial}{\partial p} \left[ \nabla^2 T_m(x, t) \right] \quad (13)
\]

where

\[
\alpha = \frac{c_{al} T_x - c_{al} T_s}{T_x - T_s} + \frac{(c_{al} - c_s) T_x T_s (T_x + T_s)}{(T_x - T_s)^3} + \frac{30 T_x^2 T_s^2 Q_m}{(T_x - T_s)^3} + \frac{30 T_x^2 T_s^2 Q_m}{(T_x - T_s)^3} + \frac{60 T_x T_s (T_x + T_s) Q_m}{(T_x - T_s)^3} + \frac{3 (c_{al} - c_s) (T_x + T_s)}{(T_x - T_s)^3} + \frac{30 (T_x^2 + 4 T_s T_s + T_s^2) Q_m}{(T_x - T_s)^3}
\]
Differentiation of substitute thermal capacity with respect to the parameters \( p_1, p_2, p_3 \) leads to the following formulas

\[
\frac{\partial C(T)}{\partial p_1} = \begin{cases} 
0, & T \geq T_L \\
\frac{\partial a_1}{\partial p_1} T + \frac{\partial a_2}{\partial p_1} T^2 + \frac{\partial a_3}{\partial p_1} T^3 + \frac{\partial a_4}{\partial p_1} T^4, & T_A \leq T < T_L \\
0, & T_L \leq T < T_A \\
0, & T < T_L 
\end{cases}
\]

(16)

and

\[
\frac{\partial C(T)}{\partial p_2} = \begin{cases} 
0, & T \geq T_I \\
\frac{1}{T_A - T_E}, & T_E \leq T < T_A \\
0, & T_A \leq T < T_E \\
0, & T < T_A 
\end{cases}
\]

(17)

while

\[
\frac{\partial C(T)}{\partial p_3} = \begin{cases} 
0, & T \geq T_E \\
\frac{\partial b_2}{\partial p_3} T + \frac{\partial b_3}{\partial p_3} T^2, & T_A \leq T < T_E \\
0, & T_E \leq T < T_A \\
0, & T < T_E 
\end{cases}
\]

(18)

Taking into account the dependences (6), (7), the calculations of \( \partial a_1/\partial p_1 \) and \( \partial b_2/\partial p_3 \) are very simple.

The boundary initial problems (14) are coupled with the basic one (8) – (12), because in order to find their solutions, the time derivative \( \partial T(x, t)/\partial t \) should be known.

The basic problem for the assumed values of \( p_1, p_2, p_3 \) 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. Gradient method

In order to solve the inverse problem the least squares criterion is applied [2, 4]

\[
S(\bar{p}_1, \bar{p}_2, \bar{p}_3) = \frac{1}{MF} \sum_{i=1}^{M} \sum_{j=1}^{F} (T_i - T_i')^2
\]

(19)

where \( T_i \) and \( T_i' \) are the measured and estimated temperatures, respectively. The estimated temperatures are obtained from the solution of the direct problem (c.f. chapter 3) by using the current available estimate for the unknown parameters.

In the case of typical gradient method application [2, 4, 6, 8] the criterion (19) is differentiated with respect to the unknown parameters \( \bar{p}_e, e = 1, 2, 3 \) and next the necessary condition of optimum is used. Finally one obtains the following system of equations

\[
\frac{\partial S}{\partial \bar{p}_e} = \frac{2}{MF} \sum_{i=1}^{M} \sum_{j=1}^{F} \left( T_i' - T_i \right) (Z_i'^{\dagger}) = 0
\]

(20)

where

\[
(Z_i'^{\dagger}) = \frac{\partial T_i'}{\partial \bar{p}_e}
\]

(21)

are the sensitivity coefficients, \( k \) is the number of iteration, \( \bar{p}_e^k \) are the arbitrary assumed values of \( p_e \), while \( \bar{p}_e^{k+1} \) for \( k > 0 \) result from the previous iteration.

The coefficients (21) can be collected in the following matrix

\[
Z^k = \begin{bmatrix} 
(Z_1^k) & (Z_2^k) & (Z_3^k) \\
\vdots & \vdots & \vdots \\
(Z^F_1) & (Z^F_2) & (Z^F_3) \\
\end{bmatrix}
\]

(22)

Function \( T_i' \) is expanded in a Taylor series about known values of \( p_i^j \), this means

\[
T_i' = \left( T_i' \right)^{\dagger} + \sum_{j=1}^{k} \left( Z_i'^{\dagger} \right) \left( p_i^{k+1} - p_i^k \right)
\]

(23)
Putting (23) into (20) one obtains ($e = 1, 2, 3$)

$$\sum_{i=1}^{M} \sum_{j=1}^{N} \left( Z_{ij}^e \right)^k (Z_{ij}^e)^{(p_{e^{k+1}} - p_{e}^k)} =$$

$$\sum_{i=1}^{M} \sum_{j=1}^{N} \left[ T_{di}^e - (T_{di}^e)^k \right] (Z_{ij}^e)^k$$

(24)

The system of equations (24) can be written in the matrix form

$$\begin{bmatrix} (Z^1)^T \end{bmatrix} \begin{bmatrix} Z^1 \end{bmatrix} P^{k+1} = \begin{bmatrix} (Z^1)^T \end{bmatrix} Z^1 P^k + \begin{bmatrix} (Z^1)^T \end{bmatrix} (T_d - T^i)$$

(25)

where

$$T_d = \begin{bmatrix} T_{d1}^1 & \cdots & T_{d1}^N \\ \vdots & \ddots & \vdots \\ T_{dM}^1 & \cdots & T_{dM}^N \end{bmatrix}, \quad T^k = \begin{bmatrix} \left(T_1^1\right)^k \\ \vdots \\ \left(T_1^N\right)^k \end{bmatrix}$$

(26)

and

$$P = \begin{bmatrix} p_1^1 \\ p_2^1 \\ p_3^1 \end{bmatrix}, \quad P^{k+1} = \begin{bmatrix} p_1^{k+1} \\ p_2^{k+1} \\ p_3^{k+1} \end{bmatrix}$$

(27)

This system of equations allows to find the values of $p_{e^{k+1}}$ for $e = 1, 2, 3$. The iteration process is stopped when the assumed number of iterations $K$ is achieved.

6. Results of computations

The casting-mould system shown in Figure 3 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)], $Q_{\text{melt}} = 937.2$ [MJ/m$^3$], $Q_{\text{ref}} = 397.6$ [MJ/m$^3$], $Q_{\text{melt}} = 582.2$ [MJ/m$^3$], $c_m = 1.75$ [MJ/(m$^3$K)], pouring temperature $T_0 = 1300$ ºC, liquidus temperature $T_L = 1250$ ºC, border temperatures $T_1 = 1200$ ºC, $T_2 = 1130$ ºC, solidus temperature $T_s = 1110$ ºC and initial mould temperature $T_m = 20$ ºC.

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].
On the basis of knowledge of cooling curves shown in Figure 4 the unknown parameters have been identified under the assumption that $Q_{aus1}^0 = Q_{aus2}^0 = Q_{eu}^0 = 0$ – Fig. 6. It is visible that the iteration process for the assumed initial values is convergent and the exact solution is obtained after twenty iterations. Figure 7 illustrates the course of iteration process for one sensor (point 1 in Fig. 3) and the same initial values of parameters.

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References