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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 [1, 2, 3]. To identify the latent heats corresponding to austenite and eutectic phases the gradient methods have been used [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 Zl200-Zl250 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 $T_d(t) = T(x_d, t)$ 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

$$\int_{T_S}^{T_L} C(T)dT = c_P\left(T_L - T_S\right) + Q \tag{1}$$

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

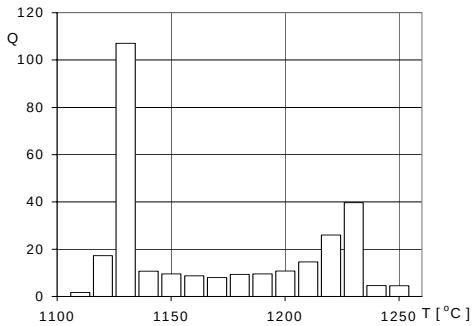

Fig. 1. Distribution of cast iron latent heat

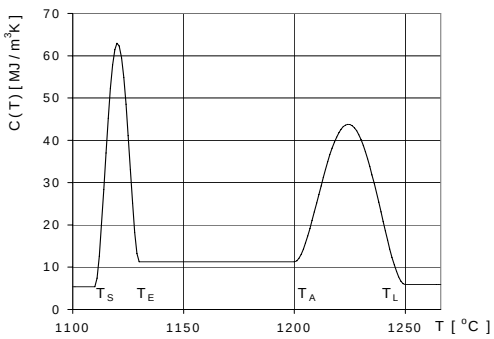

Fig. 2. Substitute thermal capacity of cast iron

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

$$C(T) = \begin{cases} c_L, & T \geq T_L \\ a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4, & T_A \leq T < T_L \\ c_{AE}, & T_E \leq T < T_A \\ b_1 + b_2T + b_3T^2 + b_4T^3 + b_5T^4, & T_S \leq T < T_E \\ c_S, & T < T_S \end{cases} \tag{2}$$

where T_L, T_A, T_E, T_S correspond to the border temperatures, a_k, b_k, $k = 1, 2, 3, 4, 5$ are the coefficients and

$$c_{AE} = c_P + \frac{Q_{aus2}}{T_A - T_E} \tag{3}$$

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

$$\begin{cases} C(T_L) = c_L \\ C(T_A) = c_{AE} \\ \left.\dfrac{\mathrm{d}C(T)}{\mathrm{d}T}\right|_{T=T_L} = 0 \\ \left.\dfrac{\mathrm{d}C(T)}{\mathrm{d}T}\right|_{T=T_A} = 0 \\ \displaystyle\int_{T_A}^{T_L} C(T)\,\mathrm{d}T = c_P\left(T_L - T_A\right) + Q_{aus1} \end{cases} \tag{4}$$

and

$$\begin{cases} C(T_E) = c_{AE} \\ C(T_S) = c_S \\ \left.\dfrac{\mathrm{d}C(T)}{\mathrm{d}T}\right|_{T=T_E} = 0 \\ \left.\dfrac{\mathrm{d}C(T)}{\mathrm{d}T}\right|_{T=T_S} = 0 \\ \displaystyle\int_{T_S}^{T_E} C(T)\,\mathrm{d}T = c_P\left(T_E - T_S\right) + Q_{eu} \end{cases} \tag{5}$$

After the mathematical manipulations one has

$$\begin{aligned} a_1 &= \frac{c_{AE}T_L - c_LT_A}{T_L - T_A} + \frac{\left(c_L - c_{AE}\right)T_LT_A\left(T_L + T_A\right)}{\left(T_L - T_A\right)^3} + \frac{30T_L^2T_A^2Q_{aus1}}{\left(T_L - T_A\right)^5} \\ a_2 &= -\frac{6\left(c_L - c_{AE}\right)T_LT_A}{\left(T_L - T_A\right)^3} - \frac{60T_LT_A\left(T_L + T_A\right)Q_{aus1}}{\left(T_L - T_A\right)^5} \\ a_3 &= \frac{3\left(c_L - c_{AE}\right)\left(T_L + T_A\right)}{\left(T_L - T_A\right)^3} + \frac{30\left(T_L^2 + 4T_LT_A + T_A^2\right)Q_{aus1}}{\left(T_L - T_A\right)^5} \\ a_4 &= -\frac{2\left(c_L - c_{AE}\right)}{\left(T_L - T_A\right)^3} - \frac{60\left(T_L + T_A\right)Q_{aus1}}{\left(T_L - T_A\right)^5} \\ a_5 &= \frac{30Q_{aus1}}{\left(T_L - T_A\right)^5} \end{aligned} \tag{6}$$

and

$$
\begin{aligned}
b_1 &= \frac{c_S T_E - c_{AE} T_S}{T_E - T_S} + \frac{(c_{AE} - c_S) T_E T_S (T_E + T_S)}{(T_E - T_S)^3} + \\
&\quad \frac{30 T_E^2 T_S^2 Q_{eu}}{(T_E - T_S)^5} \\
b_2 &= -\frac{6(c_{AE} - c_S) T_E T_S}{(T_E - T_S)^3} - \frac{60 T_E T_S (T_E + T_S) Q_{eu}}{(T_E - T_S)^5} \\
b_3 &= \frac{3(c_{AE} - c_S)(T_E + T_S)}{(T_E - T_S)^3} + \frac{30(T_E^2 + 4T_E T_S + T_S^2) Q_{eu}}{(T_E - T_S)^5} \\
b_4 &= -\frac{2(c_{AE} - c_S)}{(T_E - T_S)^3} - \frac{60(T_E + T_S) Q_{eu}}{(T_E - T_S)^5} \\
b_5 &= \frac{30 Q_{eu}}{(T_E - T_S)^5}
\end{aligned}
\tag{7}
$$

3. Governing equations

The energy equation describing the casting solidification has the following form [1, 8, 9, 10]

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

where $C(T)$ is the substitute thermal capacity of cast iron (c.f. equation (2)), λ 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

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

where c_m is the mould volumetric specific heat, λ_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

$$
x \in \Gamma_c: \quad \begin{cases} -\lambda \mathbf{n} \cdot \nabla T(x, t) = -\lambda_m \mathbf{n} \cdot \nabla T_m(x, t) \\ T(x, t) = T_m(x, t) \end{cases} \tag{10}
$$

can be accepted.

On the external surface of the system the Robin condition

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

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

For time $t = 0$ the initial condition

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

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

$$
\begin{aligned}
& x \in \Omega: \ \frac{\partial C(T)}{\partial p_e} \frac{\partial T(x, t)}{\partial t} + C(T) \frac{\partial}{\partial p_e} \left(\frac{\partial T(x, t)}{\partial t} \right) = \\
& \quad \lambda \frac{\partial}{\partial p_e} \left[\nabla^2 T(x, t) \right] \\
& x \in \Omega_m: c_m \frac{\partial}{\partial p_e} \left(\frac{\partial T_m(x, t)}{\partial t} \right) = \lambda_m \frac{\partial}{\partial p_e} \left[\nabla^2 T_m(x, t) \right] \\
& x \in \Gamma_c: \ \begin{cases} -\lambda \mathbf{n} \cdot \frac{\partial}{\partial p_e} \left[\nabla T(x, t) \right] = -\lambda_m \mathbf{n} \cdot \frac{\partial}{\partial p_e} \left[\nabla T_m(x, t) \right] \\ \frac{\partial T(x, t)}{\partial p_e} = \frac{\partial T_m(x, t)}{\partial p_e} \end{cases} \\
& x \in \Gamma_0: -\lambda_m \mathbf{n} \cdot \frac{\partial}{\partial p_e} \left[\nabla T_m(x, t) \right] = 0 \\
& t = 0: \ \frac{\partial T(x, 0)}{\partial p_e} = 0 \ , \ \frac{\partial T_m(x, 0)}{\partial p_e} = 0
\end{aligned}
\tag{13}
$$

or

$$
\begin{aligned}
& x \in \Omega: C(T) \frac{\partial Z_e(x, t)}{\partial t} = \lambda \nabla^2 Z_e(x, t) - \frac{\partial C(T)}{\partial p_e} \frac{\partial T(x, t)}{\partial t} \\
& x \in \Omega_m: c_m \frac{\partial Z_{me}(x, t)}{\partial t} = \lambda_m \nabla^2 Z_{me}(x, t) \\
& x \in \Gamma_c: \ \begin{cases} -\lambda \mathbf{n} \cdot \nabla Z_e(x, t) = -\lambda_m \mathbf{n} \cdot \nabla Z_{me}(x, t) \\ Z_e(x, t) = Z_{me}(x, t) \end{cases} \\
& x \in \Gamma_0: -\lambda_m \mathbf{n} \cdot \nabla Z_{me}(x, t) = 0 \\
& t = 0: \ Z_e(x, 0) = 0 \ , \ Z_{me}(x, 0) = 0
\end{aligned}
\tag{14}
$$

where

$$Z_e(x,t)=\frac{\partial T(x,t)}{\partial p_e}$$
$$Z_{me}(x,t)=\frac{\partial T_m(x,t)}{\partial p_e} \tag{15}$$

and $e = 1, 2, 3$.

Differentiation of substitute thermal capacity with respect to the parameters p_1, p_2, p_3 leads to the following formulas

$$\frac{\partial C(T)}{\partial p_1}=\begin{cases}0, & T\ge T_L\\ \frac{\partial a_1}{\partial p_1}+\frac{\partial a_2}{\partial p_1}T+ & \\ \frac{\partial a_3}{\partial p_1}T^2+\frac{\partial a_4}{\partial p_1}T^3+\frac{\partial a_5}{\partial p_1}T^4+ & T_A\le T<T_L\\ \left(a_2+2a_3T+3a_4T^2+4a_5T^3\right)Z_1, & \\ 0, & T_E\le T<T_A\\ 0, & T_S\le T<T_E\\ 0, & T<T_S\end{cases} \tag{16}$$

and

$$\frac{\partial C(T)}{\partial p_2}=\begin{cases}0, & T\ge T_L\\ 0, & T_A\le T<T_L\\ \frac{1}{T_A-T_E}, & T_E\le T<T_A\\ 0, & T_S\le T<T_E\\ 0, & T<T_S\end{cases} \tag{17}$$

while

$$\frac{\partial C(T)}{\partial p_3}=\begin{cases}0, & T\ge T_L\\ 0, & T_A\le T<T_L\\ 0, & T_E\le T<T_A\\ \frac{\partial b_1}{\partial p_3}+\frac{\partial b_2}{\partial p_3}T+ & \\ \frac{\partial b_3}{\partial p_3}T^2+\frac{\partial b_4}{\partial p_3}T^3+\frac{\partial b_5}{\partial p_3}T^4+ & T_S\le T<T_E\\ \left(b_2+2b_3T+3b_4T^2+4b_5T^3\right)Z_3, & \\ 0, & T<T_S\end{cases} \tag{18}$$

Taking into account the dependences (6), (7), the calculations of $\partial a_k/\partial p_1$ and $\partial b_k/\partial p_3$ 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]

$$S\left(p_1, p_2, p_3\right)=\frac{1}{MF}\sum_{i=1}^{M}\sum_{f=1}^{F}\left(T_i^f-T_{di}^f\right)^2 \tag{19}$$

where T_{di}^f and $T_i^f = T(x_i, t^f)$ 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 p_e, $e = 1, 2, 3$ and next the necessary condition of optimum is used. Finally one obtains the following system of equations

$$\frac{\partial S}{\partial p_e}=\frac{2}{MF}\sum_{i=1}^{M}\sum_{f=1}^{F}\left(T_i^f-T_{di}^f\right)\left(Z_{ie}^f\right)^k=0 \tag{20}$$

where

$$\left(Z_{ie}^f\right)^k=\left.\frac{\partial T_i^f}{\partial p_e}\right|_{p_e=p_e^k} \tag{21}$$

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.

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

$$\mathbf{Z}^k=\begin{bmatrix}\left(Z_{11}^1\right)^k & \left(Z_{12}^1\right)^k & \left(Z_{13}^1\right)^k\\ \cdots & \cdots & \cdots\\ \left(Z_{11}^F\right)^k & \left(Z_{12}^F\right)^k & \left(Z_{13}^F\right)^k\\ \left(Z_{21}^1\right)^k & \left(Z_{22}^1\right)^k & \left(Z_{23}^1\right)^k\\ \cdots & \cdots & \cdots\\ \left(Z_{21}^F\right)^k & \left(Z_{22}^F\right)^k & \left(Z_{23}^F\right)^k\\ \cdots & \cdots & \cdots\\ \left(Z_{M1}^1\right)^k & \left(Z_{M2}^1\right)^k & \left(Z_{M3}^1\right)^k\\ \cdots & \cdots & \cdots\\ \left(Z_{M1}^F\right)^k & \left(Z_{M2}^F\right)^k & \left(Z_{M3}^F\right)^k\end{bmatrix} \tag{22}$$

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

$$T_i^f=\left(T_i^f\right)^k+\sum_{l=1}^{3}\left(Z_{il}^f\right)^k\left(p_l^{k+1}-p_l^k\right) \tag{23}$$

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

$$\sum_{i=1}^{M}\sum_{f=1}^{F}\sum_{l=1}^{3}\left(Z_{il}^{f}\right)^{k}\left(Z_{ie}^{f}\right)^{k}\left(p_{l}^{k+1}-p_{l}^{k}\right)= \sum_{i=1}^{M}\sum_{f=1}^{F}\left[T_{di}^{f}-\left(T_{i}^{f}\right)^{k}\right]\left(Z_{ie}^{f}\right)^{k} \tag{24}$$

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

$$\left(\mathbf{Z}^{k}\right)^{\mathrm{T}}\mathbf{Z}^{k}\mathbf{p}^{k+1}=\left(\mathbf{Z}^{k}\right)^{\mathrm{T}}\mathbf{Z}^{k}\mathbf{p}^{k}+\left(\mathbf{Z}^{k}\right)^{\mathrm{T}}\left(\mathbf{T}_{d}-\mathbf{T}^{k}\right) \tag{25}$$

where

$$\mathbf{T}_{\mathrm{d}}=\begin{bmatrix} T_{d\,1}^{1} \\ \cdots \\ T_{d\,1}^{F} \\ T_{d\,2}^{1} \\ \cdots \\ T_{d\,2}^{F} \\ \cdots \\ T_{d\,M}^{1} \\ \cdots \\ T_{d\,M}^{F} \end{bmatrix}, \qquad \mathbf{T}^{k}=\begin{bmatrix} \left(T_{1}^{1}\right)^{k} \\ \cdots \\ \left(T_{1}^{F}\right)^{k} \\ \left(T_{2}^{1}\right)^{k} \\ \cdots \\ \left(T_{2}^{F}\right)^{k} \\ \cdots \\ \left(T_{M}^{1}\right)^{k} \\ \cdots \\ \left(T_{M}^{F}\right)^{k} \end{bmatrix} \tag{26}$$

and

$$\mathbf{p}^{k}=\begin{bmatrix} p_{1}^{k} \\ p_{2}^{k} \\ p_{3}^{k} \end{bmatrix}, \qquad \mathbf{p}^{k+1}=\begin{bmatrix} p_{1}^{k+1} \\ p_{2}^{k+1} \\ p_{3}^{k+1} \end{bmatrix} \tag{27}$$

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)], $Q_{aus1} = 937.2$ [MJ/m^3], $Q_{aus2} = 397.6$ [MJ/m^3], $Q_{eu} = 582.2$ [MJ/m^3], $c_m = 1.75$ [MJ/(m^3 K)], pouring temperature $T_0 = 1300$ ° C, liquidus temperature $T_L = 1250$ ° C, border temperatures $T_A = 1200$ ° C, $T_E = 1130$ ° C, solidus temperature $T_S = 1110$ ° C and initial mould temperature $T_{m0} = 20$ ° C.

The direct problem has been solved using the explicit scheme of FDM [1]. The regular mesh created by 25×15 nodes with constant step $h = 0.002$ [m] has been introduced, time step $\Delta t = 0.1$ [s].

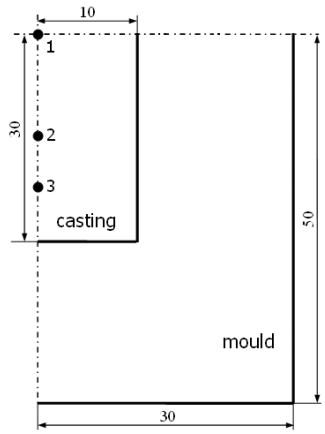

Fig. 3. Casting-mould system

In Figure 4 the cooling curves at the control points 1, 2, 3 from casting sub-domain (c.f. Fig. 3) are shown, while Figure 5 illustrates the courses of sensitivity functions Z_e at the point 1.

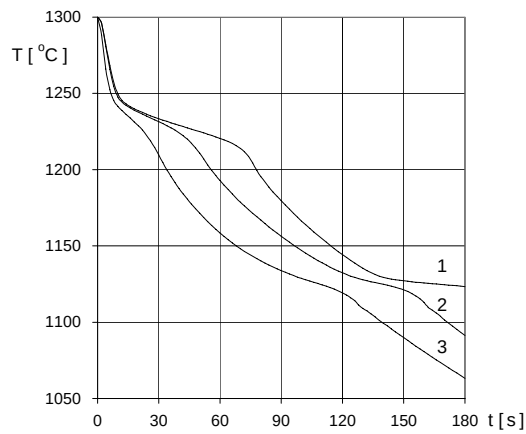

Fig. 4. Cooling curves at the points 1, 2, 3

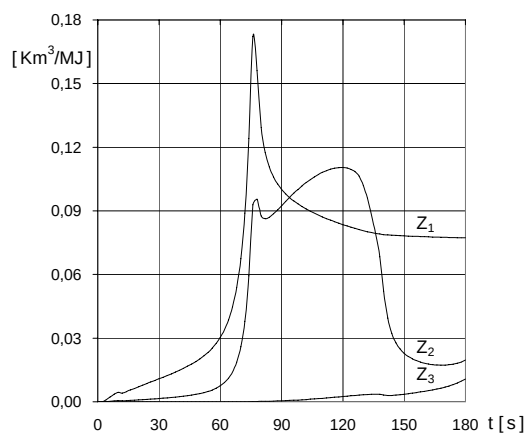

Fig. 5. Sensitivity functions at the point 1

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.

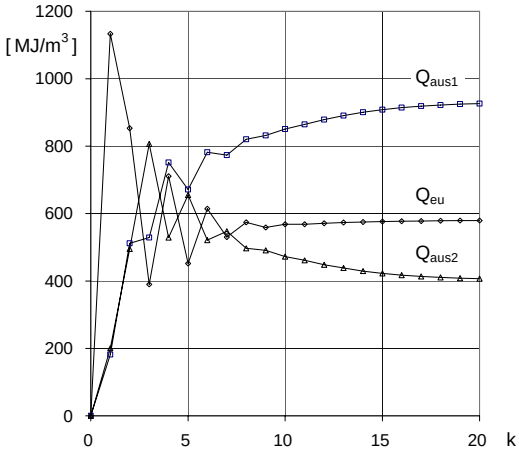

Fig. 6. Result of identification for three cooling curves

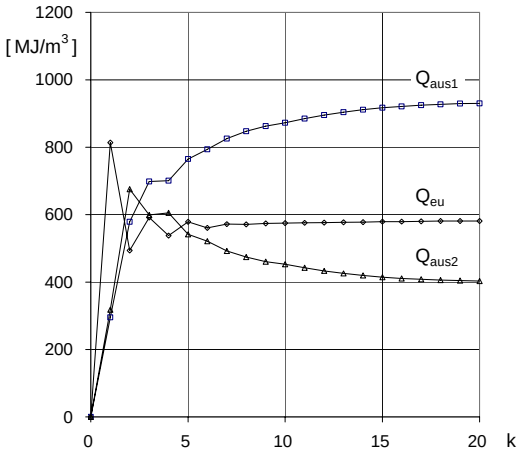

Fig. 7. Result of identification for one cooling curve

7. Conclusions

The testing computations show that it is possible to identify the unknown parameters only on the basis of one cooling curve knowledge but it should be located at the central part of the casting domain. In this case for zero initial values of identified parameters the iterative process is convergent.

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