IDENTIFICATION OF SOLIDIFICATION MODEL PARAMETERS

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Abstract. In the paper the parametric inverse problem [1, 2] concerning the identification of latent heat is considered. This parameter appears in the energy equation in the source term if the one domain approach is taken into account [4]. The identification of latent heat is possible under the condition that one disposes the additional information concerning the temperature field in the casting domain (cooling curves at the selected set of points). In order to solve the problem the algorithm using the sensitivity coefficients and least squares criterion has been used. The numerical example is presented in the final part of the paper.

1. Formulation of the problem

The casting-mould system $\Omega = \Omega_1 \cup \Omega_2$ is considered. Let us assume that the one-dimensional transient temperature field in the casting domain Ω_1 is described by the equation concerning only conductional heat transfer (the convection is neglected). Then

$$x \in \Omega_1 \quad : \quad c_1 \frac{\partial T(x,t)}{\partial t} = \lambda_1 \frac{\partial^2 T(x,t)}{\partial x^2} + L \frac{\partial f_S}{\partial t} \tag{1}$$

where c_1, λ_1 denote volumetric specific heat and a thermal conductivity, $T(x,t)$ is a temperature, L denotes a volumetric latent heat, f_S is a solid state fraction at the neighborhood of considered point from casting domain, x, t denote the spatial co-ordinates and time.

The temperature field in the mould domain Ω_2 is described by the equation

$$x \in \Omega_2 \quad : \quad c_2 \frac{\partial T(x,t)}{\partial t} = \lambda_2 \frac{\partial^2 T(x,t)}{\partial x^2} \tag{2}$$

where c_2, λ_2 denote volumetric specific heat and a thermal conductivity.

The following boundary-initial conditions are assumed

$$x \in \Gamma_1 \quad : \quad -\lambda_1 \frac{\partial T(x,t)}{\partial x} = q_b \tag{3}$$

$$x \in \Gamma_2 \quad : \quad -\lambda_2 \frac{\partial T(x,t)}{\partial x} = \alpha\left(T(x,t) - T_a\right) \tag{4}$$

$$x \in \Gamma_3 \quad : \quad -\lambda_1 \frac{\partial T_1(x,t)}{\partial x} = \frac{T_1 - T_2}{R} = -\lambda_2 \frac{\partial T_2(x,t)}{\partial x} \tag{5}$$

$$t = 0 \quad : \quad T(x,t) = T_0(x) \tag{6}$$

where $\partial/\partial n$ is a normal derivative, q_b is a boundary heat flux, α is a heat transfer coefficient, T_a denotes an ambient temperature, R is a thermal contact resistance, T_0 denotes an initial temperature distribution.
It is assumed that f_S is a known temperature-dependent function from the scope [0,1]. Then

$$\frac{\partial f_S}{\partial t} = \frac{\mathrm{d} f_S}{\mathrm{d} T} \frac{\partial T(x,t)}{\partial t} \tag{7}$$

and equation (1) can be written in the form

$$\left[c_1(T) - L \frac{\mathrm{d} f_S}{\mathrm{d} T}\right] \frac{\partial T(x,t)}{\partial t} = \lambda_1 \frac{\partial^2 T(x,t)}{\partial x^2} \tag{8}$$

Parameter

$$C(T) = c_1(T) - L \frac{\mathrm{d} f_S}{\mathrm{d} T} \tag{9}$$

is called the substitute thermal capacity. Because the new equation

$$C(T) \frac{\partial T(x,t)}{\partial t} = \lambda_1 \frac{\partial^2 T(x,t)}{\partial x^2} \tag{10}$$

concerns the whole conventionally homogenized casting domain therefore this approach is called one domain method or fixed domain method [4]. If T_L and T_S denote the temperatures corresponding to the beginning and the end of solidification then

$$C(T) = \begin{cases} c_L & , \quad T > T_L \\ c_P - L \dfrac{df_S}{dT} & , \quad T_S \le T \le T_L \\ c_S & , \quad T < T_S \end{cases} \tag{11}$$

where c_L, c_P, c_S are the volumetric specific heats of molten metal, mushy zone and solidified part of casting. In literature (e.g. [4]) one can find the different formulas determining the mushy zone thermal capacity. In this paper we used the function

$$C(T) = c_S + \left(c_{\max} - c_S\right) \frac{T - T_S}{T_L - T_S} \quad , \quad T \in \left[T_S, T_L\right] \tag{12}$$

where

$$c_{\max} = 2c_P + c_S + \frac{2L}{T_L - T_S} \tag{13}$$

There are also known 'measured' temperatures at the selected set of M control points

$$T\left(x^i, t^f\right) = T_{di}^f \ , \ i = 1, 2, \dots, M \ \text{ and } \ f = 1, 2, \dots, F \tag{14}$$

The problem consists in the calculation of unknown latent heat L.

2. Identification of latent heat

Let Z denotes the sensitivity function [1, 2] $Z = \partial T/\partial L$. Distribution of this function results from the solution of the following boundary-initial problem

$$x \in \Omega_1 \quad : \quad C\frac{\partial Z(x,t)}{\partial t} = \lambda_1 \frac{\partial^2 Z(x,t)}{\partial x^2} - \frac{\partial C}{\partial L}\frac{\partial T(x,t)}{\partial t} \tag{15}$$

$$x \in \Omega_2 \quad : \quad c_2 \frac{\partial Z(x,t)}{\partial t} = \lambda_2 \frac{\partial^2 Z(x,t)}{\partial x^2} \tag{16}$$

$$x \in \Gamma_1 \quad : \quad -\lambda_1 \frac{\partial Z(x,t)}{\partial x} = 0 \tag{17}$$

$$x \in \Gamma_2 \quad : \quad -\lambda_2 \frac{\partial Z(x,t)}{\partial x} = \alpha Z \tag{18}$$

$$x \in \Gamma_3 \quad : \quad -\lambda_1 \frac{\partial Z_1(x,t)}{\partial x} = \frac{Z_1 - Z_2}{R} = -\lambda_2 \frac{\partial Z_2(x,t)}{\partial x} \tag{19}$$

$$t = 0 \quad : \quad Z(x,t) = 0 \tag{20}$$

Because the temperature field is continuous one it can be expanded in a Taylor series about an arbitrary but known value L^k

$$T_i^f = \left(T_i^f\right)^k + \left.\frac{\partial T_i^f}{\partial L}\right|_{L=L^k} \left(L^{k+1} - L^k\right) \tag{21}$$

where k is the index of iteration.
Thus

$$T_i^f = \left(T_i^f\right)^k + \left(Z_i^f\right)^k \left(L^{k+1} - L^k\right) \tag{22}$$

where $Z_i^f = Z\left(x^i, t^f\right)$.

The least squares method is used in which the sum of squares

$$S = \sum_{f=1}^{F} \sum_{i=1}^{M} \left(T_i^f - T_{di}^f\right)^2 \tag{23}$$

is minimized with respect to the parameter L.

Following the usual procedure of differentiation S with respect to L^k we obtain

$$\frac{\partial S}{\partial L} = 2 \sum_{i=1}^{M} \sum_{f=1}^{F} \left(T_i^f - T_{di}^f\right) \frac{\partial T_i^f}{\partial L} \bigg|_{L=L^k} = 0 \tag{24}$$

Substituting Eq. (22) into Eq. (24) and using simple transformations yields.

$$\sum_{i=1}^{M} \sum_{f=1}^{F} \left[\left(T_i^f\right)^k + \left(Z_i^f\right)^k \left(L^{k+1} - L^k\right) - T_{di}^f \right] \left(Z_i^f\right)^k = 0 \tag{25}$$

Eq. (21) can be written in the matrix form [2]

$$\left(\mathrm{Z}^{\mathrm{T}}\right)^k \mathrm{Z}^k \mathrm{L}^{k+1} = \left(\mathrm{Z}^{\mathrm{T}}\right)^k \mathrm{Z}^k \mathrm{L}^k + \left(\mathrm{Z}^{\mathrm{T}}\right)^k \left(\mathrm{T}_d - \mathrm{T}^k\right) \tag{26}$$

where

$$\mathrm{L}^{k+1} = \left[L^{k+1}\right],\ \mathrm{L}^k = \left[L^k\right],\ \mathrm{T}_d = \begin{bmatrix} T_{d1}^1 \\ T_{d1}^2 \\ \ldots \\ T_{d1}^F \\ T_{d2}^1 \\ T_{d2}^2 \\ \ldots \\ T_{d2}^F \\ \ldots \\ T_{dM}^1 \\ T_{dM}^2 \\ \ldots \\ T_{dM}^F \end{bmatrix},\ \mathrm{T}^k = \begin{bmatrix} \left(T_1^1\right)^k \\ \left(T_1^2\right)^k \\ \ldots \\ \left(T_1^F\right)^k \\ \left(T_2^1\right)^k \\ \left(T_2^2\right)^k \\ \ldots \\ \left(T_2^F\right)^k \\ \ldots \\ \left(T_M^1\right)^k \\ \left(T_M^2\right)^k \\ \ldots \\ \left(T_M^F\right)^k \end{bmatrix},\ \mathrm{Z}^k = \begin{bmatrix} \left(Z_1^1\right)^k \\ \left(Z_1^2\right)^k \\ \ldots \\ \left(Z_1^F\right)^k \\ \left(Z_2^1\right)^k \\ \left(Z_2^2\right)^k \\ \ldots \\ \left(Z_2^F\right)^k \\ \ldots \\ \left(Z_M^1\right)^k \\ \left(Z_M^2\right)^k \\ \ldots \\ \left(Z_M^F\right)^k \end{bmatrix} \tag{27}$$

3. Example of computation

The presented solution concerns the 1D problem. The segment Ω_1 = [0;0.05] corresponds to the sub-domain of solidifying cast iron (0.35% C), while the segment Ω_2 = [0.05;0.1] corresponds to the sub-domain of synthetic sand-mix (high-silica sand + 5% bentonite). The following thermo physical parameters are assumed for Ω_1: $\lambda_1 = 27.5$ W/mK, $L = 1984.5 \cdot 10^6$ J/m^3, $T_L = 1505^{\circ}$C, $T_S = 1470^{\circ}$C, the volumetric specific heat for solid state $c_S = 4.875 \cdot 10^6$ J/m$^3 \cdot$ K and for the liquid one $c_L = 5.292 \cdot 10^6$ J/m$^3 \cdot$ K, the initial temperature $T_0^1 = 1550^{\circ}$C.
It has been assumed that the substitute thermal capacity is in the form [3, 4]

$$C(T) = \begin{cases} 5.292 \cdot 10^6 & T > 1505 \\ -4810.464015 \cdot 10^6 + 3.2756745 \cdot 10^6 \cdot T & 1470 \le T \le 1505 \\ 4.875 \cdot 10^6 & T < 1470 \end{cases} \tag{28}$$

The parameters $p_1 = -4810.464015 \cdot 10^6$, $p_2 = 3.2756745 \cdot 10^6$ have been identified.

There have been assumed following values for sand-mix area: $\lambda_2 = 0.5$ W/mK, $c_2 = 1.639 \cdot 10^6$ J/m$^3 \cdot$ K, the initial temperature $T_0^2 = 40^{\circ}$C.

The parameters of the boundary conditions have the values: for $x = 0$: $q_b = 0$ W/m^2, for $x = 0.1$: $\alpha = 60$ W/m^{2}K, $T_a = 40^{\circ}$C, for $x = 0.5$ $R = 0$ (R is the thermal contact resistance).

Table 1

Case	Number of simulation	$\hat{L}$
1	1	269999.99997
2	2	254516
	3	276456
	4	259523
	5	258498
	6	273174
	7	279389
	8	275076
	9	268521
	10	279887
Mean value		269503.9

In numerical realization (FEM [5]) the domain Ω has been divided into 100 linear finite elements, time step $\Delta t = 1$ s. the cooling curves at five control points ($x_1 = 0.05$ m, $x_2 = 0.051$ m, $x_3 = 0.052$ m, $x_4 = 0.053$ m, $x_5 = 0.054$ m) are registered until $t = 800$ s. The results presented have been obtained for 5-th iteration (starting point $p_1^0 = 1$, $p_2^0 = 1$).
In Table 1 the results of L J/kg · K identification for undisturbed temperatures (case 1) and disturbed temperatures (case 2 - standard deviation $\sigma = 0.1$) are presented.

Conclusions

The example presented is significant from practical point of view. The identification of latent heat for solidifying casting is possible only on the basis of temperature measurements at mould locations. In these locations the values of temperature are lower and it is easier to place there thermocouples.

References

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