KINETICS OF CASTING SOLIDIFICATION - AN INVERSE APPROACH

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Abstract. In the paper the example of inverse problems application in the thermal theory of foundry processes is discussed. The solidification of typical binary alloys is considered, at the same time the macro model basing on the substitute thermal capacity is taken into account (fixed domain approach). The information necessary in order to determine the kinetics of casting solidification results from the knowledge of cooling (heating) curves at the selected set of points from casting and/or mould sub-domains. The identified value corresponds to the volumetric latent heat of alloy and, as will be shown, the knowledge of this parameter allows to determine the course of solidification, in particular the changes of temporary values of volumetric solid state fraction at the points selected from casting domain. The inverse problem considered is solved using the gradient method. On the stage of numerical simulation the FDM algorithm is used. In the final part of paper the example of computations is shown.

1. Mathematical formulation of the problems

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

$$c(T)\frac{\partial T(x,t)}{\partial t} = \nabla\left[\lambda(T)\,\nabla T(x,t)\right] + L\frac{\partial f_S(x,t)}{\partial t} \tag{1}$$

where $c(T)$ is a volumetric specific heat, $\lambda(T)$ is a thermal conductivity, L is a volumetric latent heat (this parameter is assumed to be unknown), f_S is a volumetric solid state fraction at the considered point from casting domain, T, x, t denote the temperature, geometrical co-ordinates and time. The form of equation (1) shows that only conductional heat transfer is considered and the convection in the molten metal is neglected.

Terms containing the derivatives of temperature and f_S with respect to time can be joined together and then, after the simple mathematical manipulations [1, 2], one obtains the modified form of equation (1), namely

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

where

$$C(T)=c(T)-L\frac{\mathrm{d}f_S}{\mathrm{d}T} \tag{3}$$

The function $C(T)$ is called a substitute thermal capacity [1, 2]. It should be pointed out, that the typical binary alloys solidify in an interval of temperature $\left[T_S, T_L\right]$. The sub-domain corresponding to this interval constitutes a mushy zone $f_S\in(0,1)$, for $T<T_S$: $f_S=1$ (solid state), while for $T>T_L$: $f_S=0$ (molten metal). Additionally for sub-domains of solid and liquid $\mathrm{d}f_S/\mathrm{d}T=0$ and equation (3) determines the temperature field in whole, conventionally homogeneous, casting domain. One can see, that the knowledge of temperature-dependent function f_S allows to determine the course of $C(T)$ for $T\in\left[T_S, T_L\right]$, but the other approach is also acceptable. One can assume directly the form of $C(T)$ fulfilling the condition resulting from the simple physical considerations, namely

$$\int_{T_S}^{T_L} C(T)\,\mathrm{d}T=c_P\left(T_L-T_S\right)+L \tag{4}$$

where c_P is a mushy zone volumetric specific heat (for instance $c_P=0.5\left(c_S+c_L\right)$).

Equation determining a temperature field in a mould sub-domain is the following

$$c_m(T)\frac{\partial T_m(x,t)}{\partial t}=\nabla\left[\lambda_m(T)\nabla T_m(x,t)\right] \tag{5}$$

where c_m is a mould volumetric specific heat, λ_m is a mould thermal conductivity. In the case of typical sand molds on the contact surface casting-mould the continuity of temperature and heat flux can be accepted

$$x\in\Gamma_c:\quad\begin{cases}-\lambda\dfrac{\partial T(x,t)}{\partial n}=-\lambda_m\dfrac{\partial T_m(x,t)}{\partial n}\\ T(x,t)=T_m(x,t)\end{cases} \tag{6}$$

where $\partial/\partial n$ denotes a normal derivative.

On the external surface of the system the condition in a general form

$$x \in \Gamma_0 : \quad \Phi\left[T(x, t), \frac{\partial T(x, t)}{\partial n}\right] = 0 \tag{7}$$

is given, at the same time the typical formula determining a heat exchange between mould and environment is the following

$$x \in \Gamma_0 : \quad -\lambda_m \frac{\partial T_m(x, t)}{\partial n} = \alpha\left[T_m(x, t) - T_a\right] \tag{8}$$

where α is a heat transfer coefficient, T_a is an ambient temperature. For time $t = 0$ the initial values

$$t = 0 : \quad T(x, 0) = T_0(x), \quad T_m(x, 0) = T_{m0}(x) \tag{9}$$

are also known.

2. Substitute thermal capacity

In literature one can find also the "direct" definitions of $C(T)$, in other words the form of function $C(T)$ is assumed a'priori, for example [3]

$$C(T) = a_0 + a_1 T + a_2 T^2 + a_3 T^3 + a_4 T^4, \quad T \in \left[T_S, T_L\right] \tag{10}$$

where a_e, $e = 0, 1, 2, 3, 4$ are the coefficients and they can be found on the basis of conditions assuring the continuity of C^1 class and physical correctness of approximation, namely

$$\begin{aligned} C(T_L) &= c_L \\ C(T_S) &= c_S \\ \left.\frac{\mathrm{d}C(T)}{\mathrm{d}T}\right|_{T=T_L} &= 0 \\ \left.\frac{\mathrm{d}C(T)}{\mathrm{d}T}\right|_{T=T_S} &= 0 \end{aligned} \tag{11}$$

and additionally the condition (4) must be also fulfilled.

The number of unknown parameters corresponds to the number of conditions and one can find the values of a_e, in particular [4]

$$
\begin{aligned}
a_0 &= \frac{c_S T_L - c_L T_S}{T_L - T_S} = \frac{\left(c_L - c_S\right) T_L T_S \left(T_L + T_S\right)}{\left(T_L - T_S\right)^3} + \frac{30 T_L^2 T_S^2 L}{\left(T_L - T_S\right)^5} \\
a_1 &= -\frac{6\left(c_L - c_S\right) T_L T_S}{\left(T_L - T_S\right)^3} - \frac{60 T_L T_S \left(T_L + T_S\right) L}{\left(T_L - T_S\right)^5} \\
a_2 &= \frac{3\left(c_L - c_S\right)\left(T_L + T_S\right)}{\left(T_L - T_S\right)^3} + \frac{30\left(T_L^2 + 4 T_L T_S + T_S^2\right) L}{\left(T_L - T_S\right)^5} \\
a_3 &= -\frac{2\left(c_L - c_S\right)}{\left(T_L - T_S\right)^3} - \frac{60\left(T_L + T_S\right) L}{\left(T_L - T_S\right)^5} \\
a_4 &= \frac{30 L}{\left(T_L - T_S\right)^5}
\end{aligned}
\tag{12}
$$

The course of substitute thermal capacity found using the approximation (10) for Al-Si alloy (5% Si) is shown in Figure 1.

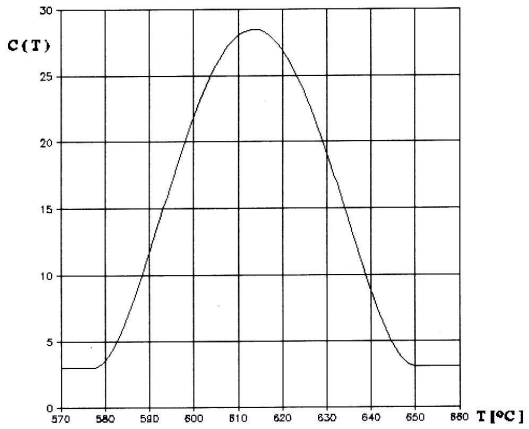

Fig. 1. Substitute thermal capacity

It is assumed that in the formula determining $C(T)$ the parameter L is unknown and the first stage of the algorithm reduces to the solution of inverse problem concerning this parameter identification. Next using the definition (3) one has

$$
c_P - L\frac{\mathrm{d}\, f_S}{\mathrm{d}T} = a_0 + a_1 T + a_2 T^2 + a_3 T^3 + a_4 T^4, \quad T \in \left[T_S, T_L\right] \tag{13}
$$

and next

$$f_S = \frac{c_P - a_0}{L} T - \frac{1}{2L} a_1 T^2 - \frac{1}{3L} a_2 T^3 - \frac{1}{4L} a_3 T^4 - \frac{1}{5L} a_4 T^5 + C \tag{14}$$

The constant C results from the condition $T = T_L$: $f_S = 0$ and finally

$$\begin{aligned} f_S = {} & \frac{a_0 - c_P}{L}\left(T_L - T\right) + \frac{1}{2L} a_1 \left(T_L^2 - T^2\right) + \frac{1}{3L} a_2 \left(T_L^3 - T^3\right) + \\ & + \frac{1}{4L} a_3 \left(T_L^4 - T^4\right) + \frac{1}{5L} a_4 \left(T_L^5 - T^5\right), \quad T \in \left[T_S, T_L\right] \end{aligned} \tag{15}$$

One can check that equation (15) fulfills the second condition, namely $T = T_S$: $f_S = 1$. The last formula determines the local and temporary value of f_S this means allows to predict the kinetics of casting solidification.

3. Inverse problem

In order to identify the value of L, the additional information connected with the course of the solidification process is necessary. So, we assume that the values $T_{d\,i}^{\,f}$ at the set of points x_i selected from the domain considered for times t^f are known

$$T_{d\,i}^{\,f} = T_d(x_i, t^f), \qquad i = 1, 2, ..., M, \qquad f = 1, 2, ..., F \tag{16}$$

Now, the least squares criterion is applied [5-7]

$$S(L) = \frac{1}{M F} \sum_{i=1}^{M} \sum_{f=1}^{F} \left(T_i^{\,f} - T_{d\,i}^{\,f}\right)^2 \tag{17}$$

where $T_i^{\,f} = T(x_i, t^f)$ is the calculated temperature at the point x_i for time t^f for arbitrary assumed value of L.

The criterion (17) is differentiated with respect to the unknown volumetric latent heat L and next the necessary condition of optimum is applied

$$\frac{\mathrm{d}S}{\mathrm{d}L} = \frac{2}{M F} \sum_{i=1}^{M} \sum_{f=1}^{F} \left(T_i^{\,f} - T_{d\,i}^{\,f}\right) \frac{\partial T_i^{\,f}}{\partial L}\bigg|_{L=L^k} = 0 \tag{18}$$

where k is the iteration number (L^k for $k = 0$ is the arbitrary assumed value of latent heat, while L^k for $k > 0$ results from the previous iteration). The function $T_i^{\,f}$ is expanded in the Taylor series using the known value of L^k, this means

$$T_i^f = \left(T_i^f\right)^k + \left.\frac{\partial T_i^f}{\partial L}\right|_{L=L^k} \left(L^{k+1} - L^k\right) \tag{19}$$

Putting (19) into (18) one has

$$\sum_{i=1}^{M}\sum_{f=1}^{F}\left[\left(Z_i^f\right)^k\right]^2\left(L^{k+1}-L^k\right) = \sum_{i=1}^{M}\sum_{f=1}^{F}\left(Z_i^f\right)^k\left[T_{di}^f - \left(T_i^f\right)^k\right] \tag{20}$$

or

$$L^{k+1} = L^k + \frac{\displaystyle\sum_{i=1}^{M}\sum_{f=1}^{F}\left(Z_i^f\right)^k\left[T_{di}^f - \left(T_i^f\right)^k\right]}{\displaystyle\sum_{i=1}^{M}\sum_{f=1}^{F}\left[\left(Z_i^f\right)^k\right]^2} \tag{21}$$

where

$$\left(Z_i^f\right)^k = \left.\frac{\partial T_i^f}{\partial L}\right|_{L=L^k} \tag{22}$$

are the sensitivity coefficients and $k = 0, 1, ..., K$.

In order to determine the sensitivity coefficients appearing in equation (21), the direct approach of sensitivity analysis can be applied. It depends on the differentiation of governing equations creating the solidification model with respect to L. So, the following additional problem connected with the sensitivity analysis should be solved

$$\begin{cases} x\in\Omega: & C(T)\dfrac{\partial Z(x,t)}{\partial t} = \lambda\nabla^2 Z(x,t) - \dfrac{\mathrm{d}C(T)}{\mathrm{d}T}Z(x,t)\dfrac{\partial T(x,t)}{\partial t} \\ x\in\Omega_m: & c_m\dfrac{\partial Z_m(x,t)}{\partial t} = \lambda_m\nabla^2 Z_m(x,t) \\ x\in\Gamma_c: & \begin{cases} -\lambda\dfrac{\partial Z(x,t)}{\partial n} = -\lambda_m\dfrac{\partial Z_m(x,t)}{\partial n} \\ Z(x,t) = Z_m(x,t) \end{cases} \\ x\in\Gamma_0: & -\lambda_m\dfrac{\partial Z_m(x,t)}{\partial n} = \alpha Z_m(x,t) \\ t=0: & Z(x,0)=0, \quad Z_m(x,0)=0 \end{cases} \tag{23}$$

This problem is strongly coupled with the basic one, because in order to find its solution, the time derivative $\partial T(x,t)/\partial t$ must be known.

4. Results of computations

The casting-core-mould system shown in Figure 2 has been considered. The following input data have been introduced (Al-Si alloy): $c_S = 2.943\ \mathrm{MJ/m^3K}$, $c_p = 3.0$, $c_L = 3.07$, $\lambda_S = 250\ \mathrm{W/mK}$, $\lambda_p = 177$, $\lambda_L = 104$, $L = 990.6\ \mathrm{MJ/m^3}$ (this value is identified during the first stage of computations).

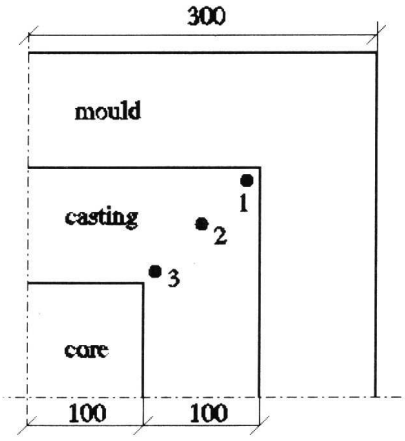

Fig. 2. Casting-mould system

Additionally it was assumed that the substitute thermal capacity of mushy zone results from formula (10). The volumetric specific heat of mould and core $c_m = 1.750\ \mathrm{MJ/m^3K}$, while the thermal conductivity $\lambda_m = 1.0$. The border and initial temperatures equal $T_S = 577^{\circ}\mathrm{C}$, $T_L = 650^{\circ}\mathrm{C}$, $T_0 = 660^{\circ}\mathrm{C}$, $T_{m0} = 20^{\circ}\mathrm{C}$. On a stage of numerical modelling the finite differences method (FDM) has been used. The casting-mould domain has been divided into 900 control volumes, time step $\Delta t = 0.001\ \mathrm{s}$. The values of "measured" temperatures result from the direct problem solution (for above collected input data) or from this solution disturbed in random way (in order to be closer to the real measurements).

In Figures 3 and 4 the cooling curves and kinetics of solidification at the points marked in Figure 2 are shown. They correspond to the real value of *L*.
Figure 5 illustrates the temperature field in the system considered for times 5 and 15 s.

The iteration process of latent heat estimation starting from the value *L* = 0 is shown in Figure 6 (undisturbed data), at the same time the values of "measured" temperature T_{di}^{f} correspond to node 3 (only one sensor has been taken into account). One can see that the number of iterations assuring the good identification is small.

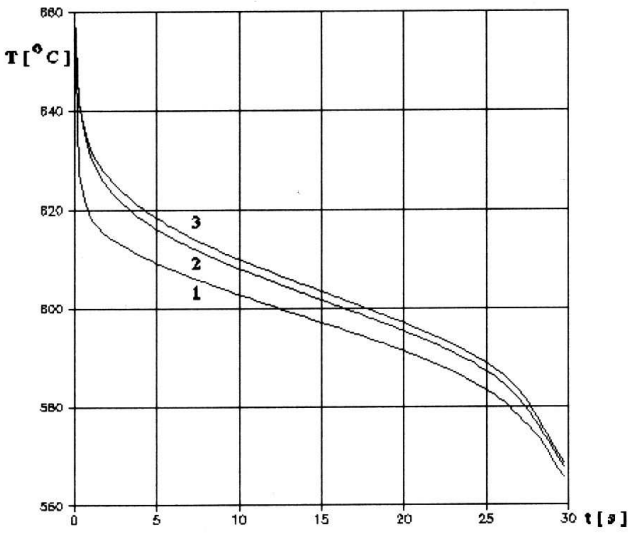

Fig. 3. Cooling curves at the points 1, 2, 3

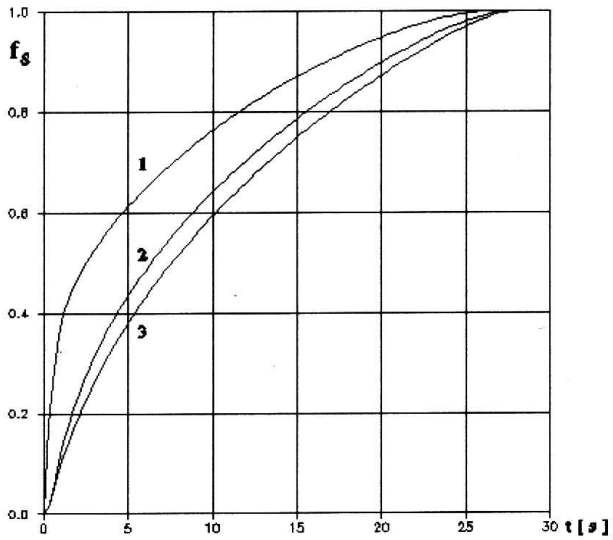

Fig. 4. Kinetics of solidification at the points 1, 2, 3

The second numerical experiment concerns the disturbed cooling curve at the point 3. The solution of direct problem is transformed in a random way and the final result is shown in Figure 7. Using this input data the good identification of latent heat has been obtained after 5 iterations. Summing up, the algorithm proposed is quite effective and exact even in the case of disturbations introduced during input data construction.

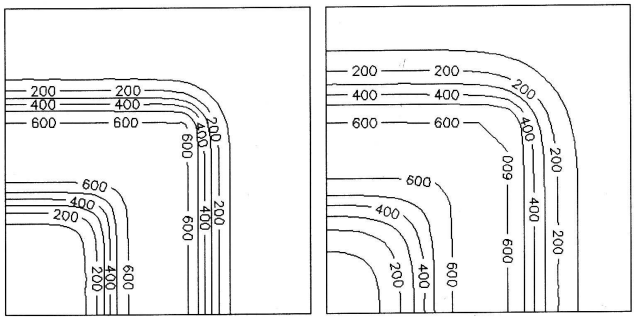

Fig. 5. Temperature distribution

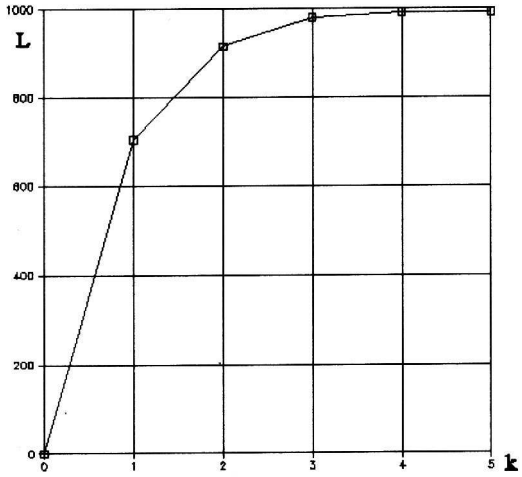

Fig. 6. Identification of latent heat

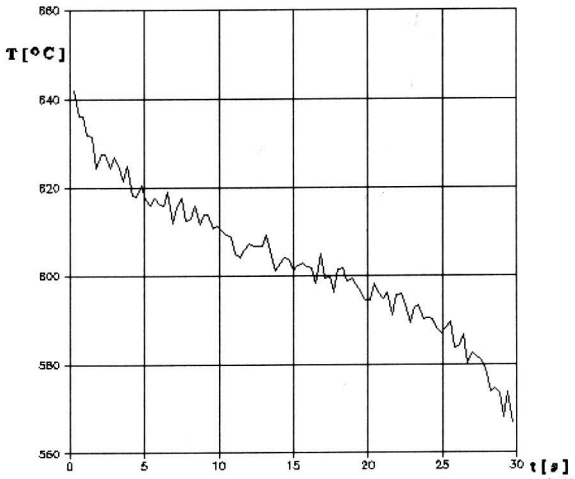

Fig. 7. Disturbed cooling curve at the point 3

Acknowledgement

The paper is connected with realization of Projects R15 008 03 and 3 T08B 004 28.

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