JOURNAL OF THEORETICAL
AND APPLIED MECHANICS
49, 4, pp. 1019-1028, Warsaw 2011

IDENTIFICATION OF ALLOY LATENT HEAT USING THE DATA OF THERMAL AND DIFFERENTIAL ANALYSIS

Bohdan Mochnacki
Romuald Szopa

Czestochowa University of Technology, Częstochowa, Poland
e-mail: moch@imi.pcz.pl

Thermal and differential analysis (TDA) is often used as a tool for quantitative estimation of solidification parameters of alloys (e.g. temperatures corresponding to the beginning and the end of phase change, kinetics of latent heat evolution, etc). TDA system offers a possibility of observation of the cooling (heating) rate, which means that the course of derivative $\partial T/\partial t$ can be analyzed. In this paper, the identification of alloy latent heat on the basis of additional information resulting from TDA measurements is discussed. At the stage of numerical modelling, the finite difference method (FDM) is used, the examples of computations are also shown.

Key words: solidification process, latent heat identification, numerical methods

1. Introduction

A typical TDA system consists of the following elements (Fig. 1):

- sample casting with thermocouple (1),
- amplifier and derivative creator (2),
- recording system and data presentation (3).

The geometry of typical sample casting is close to a cylindrical one (Mochnacki and Suchy, 1995), but in this place the other real shape of casting can also be considered, and the thermocouples can be located at the optional set of points from the domain considered. In Fig. 2, an example of TDA measurements is presented (cast iron) (Kapturkiewicz, 2003). One can see, the course of TDA curves (cooling curve and its derivative) is a smooth one, and it is a

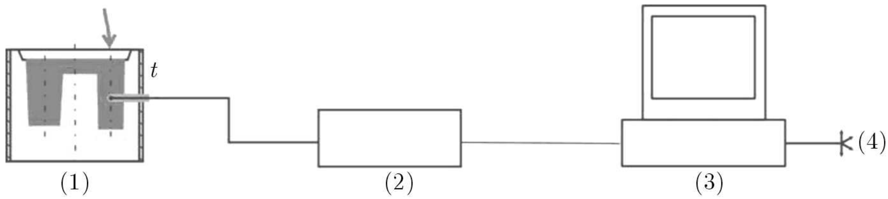

Fig. 1. TDA system

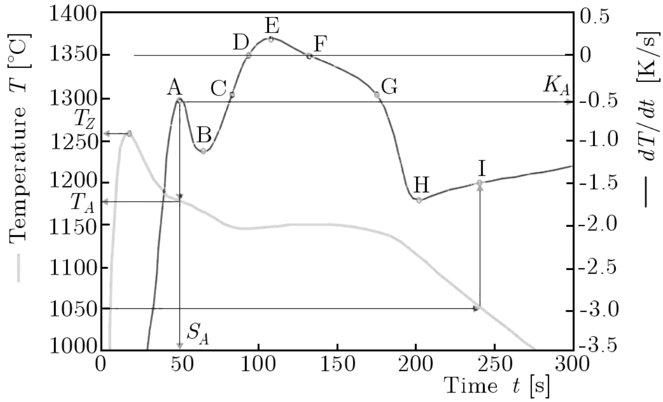

Fig. 2. Example of measured TDA curves

result of using additional numerical procedures at the stage of creation of the cooling curve and its derivative.

The position of characteristic points A, B, C,... allows one to predict different thermal and mechanical features of the casting material, but these problems will not be discussed here. The aim of considerations presented here is the identification of the alloy latent heat on the basis of information resulting from TDA measurements.

2. Mathematical description of casting solidification

The following energy equation is considered (Chang *et al.*, 1992; Kapturkiewicz, 2003; Majchrzak *et al.*, 2008; Mochnacki and Suchy, 1995)

$$c(T)\frac{\partial T(x,t)}{\partial t} = \nabla \cdot [\lambda(T)\nabla T(x,t)] + L\frac{\partial f_S(x,t)}{\partial t} \tag{2.1}$$

where $\lambda(T)$ is the thermal conductivity, $c(T)$ is the heat capacity, L is the volumetric latent heat, f_S is the volumetric solid state fraction of a metal,

$T(x,t)$, x, t denote temperature, spatial co-ordinates and time, respectively. One can see that only conductional heat transfer is taken into account (the convection is neglected) – it results from the geometrical features and dimensions of sample casting (Fig. 2). In the case of more complex thick-walled castings and considerable rates of pouring moulds (e.g. continuous casting), it is possible to apply equation (2.1), but in the place of real thermal conductivity of a molten metal, the so-called effective thermal conductivity should be introduced (see: Mochnacki and Suchy, 1995).

Assuming the knowledge of function $f_S = f_S(T)$ for the interval of temperatures $[T_S, T_L]$ corresponding to the mushy zone sub-domain, one has

$$\frac{\partial f_S(x,t)}{\partial t} = f_S'(T)\frac{\partial T(x,t)}{\partial t} \tag{2.2}$$

Additionally, for $T > T_L$: $f_S = 0$ and for $T < T_S$: $f_S = 1$, it results from the definition of the function discussed. Introducing (2.2) into (2.1) one obtains

$$[c(T) - Lf_S']\frac{\partial T(x,t)}{\partial t} = \nabla \cdot [\lambda(T)\nabla T(x,t)] \tag{2.3}$$

or

$$C(T)\frac{\partial T(x,t)}{\partial t} = \nabla \cdot [\lambda(T)\nabla T(x,t)] \tag{2.4}$$

where $C(T)$ is the substitute thermal capacity (STC) of the alloy (Kapturkiewicz, 2003; Majchrzak *et al.*, 2008; Mochnacki and Suchy, 1995). The solidification model based on equation (2.4) is called "a one-domain approach", because the same equation describes the thermal processes proceeding in the whole, conventionally homogeneous casting domain. One can see that for the molten metal and solid state, the derivative $df_S/dT = 0$ and the substitute thermal capacity directly correspond to the volumetric specific heats of these sub-domains.

One of the most popular approximation of $f_S(T)$ is the function of the form

$$f_S(T) = \Big(\frac{T_L - T(x,t)}{T_L - T_S}\Big)^n \qquad \text{for} \qquad T \in [T_S, T_L],\ n > 0 \tag{2.5}$$

Formula (2.5) assures the compliance with requirements $f_S(T_S) = 1$, $f_S(T_L) = 0$. Let us assume the linear form of function (2.5). Then, for constant values of heat capacities c_S, c_L (liquid and solid states) one obtains an approximation of $C(T)$ in the form of a stair-case function (see: definition of STC – Eq. (2.3))

$$C(T) = \begin{cases} c_L & \text{for} \quad T > T_L \\ c_P + \dfrac{L}{T_L - T_S} & \text{for} \quad T_S \leqslant T \leqslant T_L \\ c_S & \text{for} \quad T < T_S \end{cases} \tag{2.6}$$

where $c_P = 0.5(c_L + c_S)$. The parameter $L/(T_L - T_S)$ is called the spectral latent heat. In this place, more complex formulas resulting from the general form of equation (2.5) (for other values of the exponent n) can be considered, but the introduction of well known approximation (2.6) leads to a simple model determining the sensitivity coefficients W_i^f at the stage of solution of the inverse problem (see next Section). A similar formula determining the changes of casting thermal conductivity is assumed, which means

$$\lambda(T) = \begin{cases} \lambda_L & \text{for} \quad T > T_L \\ \lambda_P & \text{for} \quad T_S \leqslant T \leqslant T_L \\ \lambda_S & \text{for} \quad T < T_S \end{cases} \tag{2.7}$$

The alloy solidification and cooling process proceed in the interior of the mould. The transient heat transfer in this domain is described by the typical Fourier equation

$$c_M(T)\frac{\partial T_M(x,t)}{\partial t} = \nabla \cdot [\lambda_M(T)\nabla T_M(x,t)] \tag{2.8}$$

where $\lambda_M(T)$ is the mould thermal conductivity, $c_M(T)$ is the heat capacity of the mould. On the contact surface between the casting and mould, the condition of ideal thermal contact is assumed (continuity of temperature and heat fluxes)

$$\begin{aligned} -\lambda(T)\frac{\partial T(x,t)}{\partial n} &= -\lambda_M(T)\frac{\partial T_M(x,t)}{\partial n} \\ T(x,t) &= T_M(x,t) \end{aligned} \tag{2.9}$$

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

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

$$\Phi\Big[T_M(x,t), \frac{\partial T_M(x,t)}{\partial n}\Big] = 0 \tag{2.10}$$

is given.

The initial condition

$$t = 0: \qquad T(x,0) = T_0(x), \quad T_M(x,0) = T_{M0}(x) \tag{2.11}$$

is also known.

3. Solution to the inverse problem

To solve the inverse problem discussed, the least squares criterion of the following form is applied (Kurpisz and Nowak, 1995; Majchrzak and Mochnacki, 2007; Majchrzak *et al.*, 2007)

$$S(L) = \frac{1}{MF}\sum_{i=1}^{M}\sum_{f=1}^{F}(U_i^f - U_{di}^f)^2 = \min \tag{3.1}$$

where

$$U_i^f = \Big(\frac{\partial T}{\partial t}\Big)_i^f \qquad\qquad U_{di}^f = \Big(\frac{\partial T}{\partial t}\Big)_{di}^f \tag{3.2}$$

are the measured and estimated cooling rates, M is the number of sensors, F is the number of time levels for which the function U is determined. The estimated cooling rates are here obtained from the solution to the direct problem.

The least squares criterion used here can be treated as a special case of the criterion

$$S(L) = \frac{w}{MF}\sum_{i=1}^{M}\sum_{f=1}^{F}(T_{ri}^f - T_{rdi}^f)^2 + \frac{1-w}{MF}\sum_{i=1}^{M}\sum_{f=1}^{F}(U_{ri}^f - U_{rdi}^f)^2 = \min \tag{3.3}$$

where $T_{rd\,i}^f$ and $T_{ri}^f = T_r(x_i, t^f)$ are the measured and estimated dimensionless temperatures, U_{ri}^f, U_{rdi}^f are the measured and estimated dimensionless cooling (heating) rates, w is a tapering function $w \in [0,1]$. Effectiveness of this generalized approach will be a topic of the future research.

Using the Taylor formula, one has

$$U_i^f = (U_i^f)^k + (W_i^f)^k(L^{k+1} - L^k) \tag{3.4}$$

where

$$(W_i^f)^k = \frac{\partial U_i^f}{\partial L}\Big|_{L=L^k} \tag{3.5}$$

The necessary condition of optimum, after mathematical manipulations, leads to the formula

$$L^{k+1} = L^k + \frac{\sum\limits_{i=1}^{M}\sum\limits_{f=1}^{F}[U_{di}^f - (U_i^f)^k](W_i^f)^k}{\sum\limits_{i=1}^{M}\sum\limits_{f=1}^{F}[(W_i^f)^k]^2} \qquad k = 0, 1, 2, \dots, K \tag{3.6}$$

where k is the number of iterations and L^0 is the initial, arbitrarily assumed value of L.

To determine the sensitivity coefficients appearing in the algorithm of the inverse problem solution, one can use the method of differentiation of the governing equations with respect to the unknown parameter (the direct approach of sensitivity analysis (Dems, 1999; Kleiber, 1997; Majchrzak and Kałuża, 2008)). In the case of the problem discussed, the sensitivity model obtained in this way is rather complicated, though the approximation of $C(T)$ and $\lambda(T)$ by the stair-case functions leads to essential simplifications of this model. A more practical approach consists in the application of differential quotients (Szopa, 2006). The numerical solution of the basic model (Eqs. (2.4), (2.8)-(2.11)) allows one to directly determine the temporal and local values of the cooling (heating) rates. So, one can find the solutions to the basic problem corresponding to successive values of L^k and $L^k + \Delta L^k$, where ΔL^k is a small increase of latent heat, and next to apply the differential quotients as an approximation of the local and temporary derivatives $\partial U/\partial L$ (see Eq. (3.4)).

4. Example of computations

The symmetrical fragment of casting (steel frame) shown in Fig. 3 is considered. The casting is produced in a typical sand mould. Thermophysical parameters of the casting material are the following: $c_S = 4.875\,\mathrm{MJ/m^3K}$,

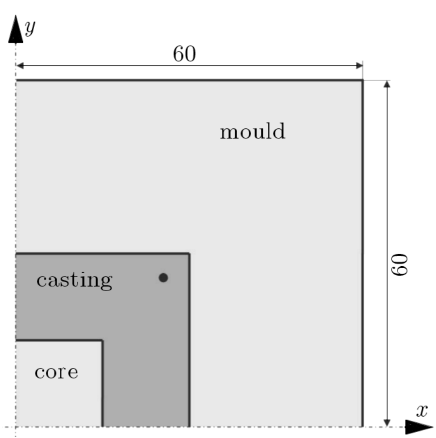

Fig. 3. Domain considered

$c_L = 5.9\,\mathrm{MJ/m^3K}$, $c_P = 5.3875\,\mathrm{MJ/m^3K}$, $L = 1984.5\,\mathrm{MJ/m^3}$ (this value is identified), $T_S = 1470°\mathrm{C}$, $T_L = 1505°\mathrm{C}$, $\lambda_S = 35\,\mathrm{W/mK}$, $\lambda_L = 20\,\mathrm{W/mK}$,

$\lambda_P = 27.5\,\mathrm{W/mK}$, while for the mould sub-domain $c_M = 1.75\,\mathrm{MJ/m^3K}$, $\lambda_M = 1\,\mathrm{W/mK}$. The initial temperature of the molten metal equals to $1550°\mathrm{C}$, initial temperature of the mould $T_{M0} = 20°\mathrm{C}$.

Both the basic and sensitivity problem have been solved using the explicit scheme of FDM for non-linear parabolic equations. Details concerning this approach to simulation of the solidification problem can be found in Mochnacki and Suchy (1995). The casting-mould domain has been discretized by a regular mesh containing 900 nodes, with the time step equal to 0.1 s.

The solution to the direct problem corresponding to the above presented input data at the point marked in Fig. 3 is shown in Fig. 4a (cooling curves) and Fig. 4b (cooling rate) – the results obtained were treated as the results of "measurements".

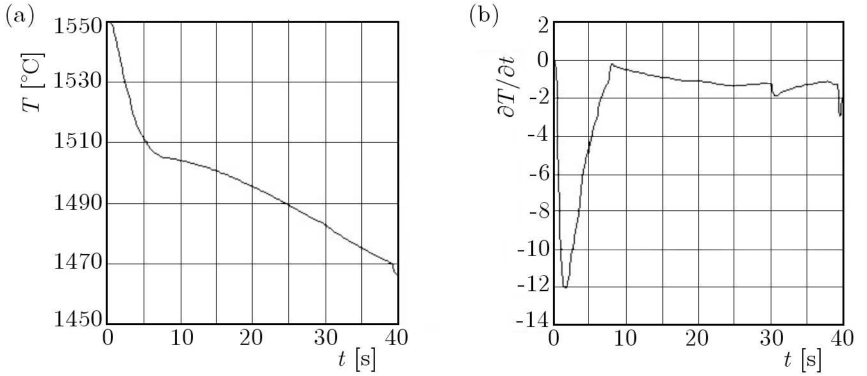

Fig. 4. (a)Cooling curve; (b) undisturbed cooling rates

The results of latent heat identification using the iteration procedure resulting from Eq. (3.6) for undisturbed input data are presented in Fig. 5.

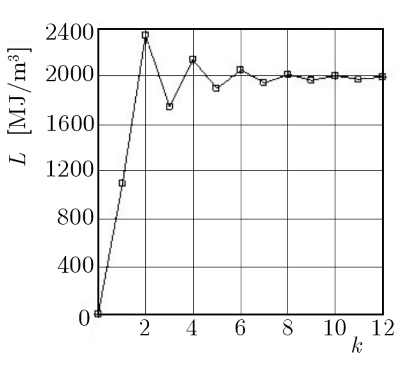

Fig. 5. Identification of L – exact data

TDA system creates, as a rule, the time derivative in form of a smooth curve (see Fig. 2b), but the inverse problem discussed has been also solved for the case of a disturbed course of this function. The randomly disturbed cooling rate at the point corresponding to the "sensor" position is shown in Fig. 6.

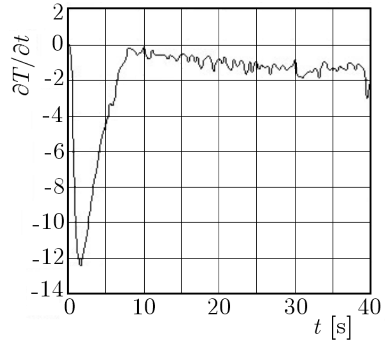

Fig. 6. Disturbed cooling rate

The identification process for the disturbed input data is presented in Fig. 7.

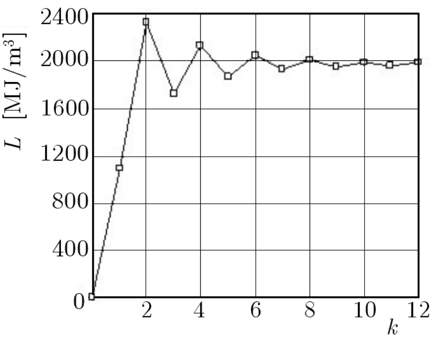

Fig. 7. Identification of L – disturbed data

5. Final remarks

The concept of cooling rate application to the solution of inverse problems results from the capability of TDA equipment. In a such case, the typical least squares criterion characteristic for gradient methods is connected with the differences between measured and calculated cooling or heating rates. The criterion assuring the optimal value of identified parameter can be generalized by the introduction of additional information concerning the temperature history (then the dimensionless temperatures and derivatives should be considered). This approach will be a subject of further research. It should be pointed out that the iteration procedure resulting from application of the gradient method is quickly convergent both in the case of undisturbed and disturbed input data – even when the distance between the starting point and the real value of the unknown parameter is considerable.

Acknowledgement
This work is a part of Research Project BS-1-105-301/99/S.

References

1. Chang S., Stefanescu D.M., Shangguan D., 1992, Modelling of the liquid/solid and eutectoid transformation in spherical graphite cast iron, *Metallurgical Transactions A*, **23A**, 1333
2. Dems K., Rousselet B., 1999, Sensitivity analysis for transient heat conduction in a solid body, *Structural Optimization*, **17**, 36-45
3. Kapturkiewicz W., 2003, *Modelling of Cast Iron Crystallization*, Cracow: AKAPIT
4. Kleiber M., 1997, *Parameter Sensitivity*, J.Wiley & Sons Ltd., Chichester
5. Kurpisz K., Nowak A., 1995, *Inverse Thermal Problems*, Southampton, Boston: Computational Mechanics Publications
6. Majchrzak E., Kałuża G., 2008, Explicit and implicit approach of sensitivity analysis in numerical modelling of solidification, *Archives of Foundry Engineering*, **8**, 1, 187-192
7. Majchrzak E., Mochnacki B., 2007, Identification of thermal properties of the system casting – mould, *Materials Science Forum*, 539-543, 2491-2496
8. Majchrzak E., Mochnacki B., Suchy J.S., 2007, Kinetics of casting solidification – an inverse approach, *Scientific Research of the Institute of Mathematics and Computer Science of Czestochowa University of Technology*, Czestochowa, **1**, 6, 169-178
9. Majchrzak E., Mochnacki B., Suchy J.S., 2008, Identification of substitute thermal capacity of solidifying alloy, *Journal of Theoretical and Applied Mechanics*, **46**, 2, 257-268

10. Mochnacki B., Suchy J.S., 1995, *Numerical Methods in Computations of Foundry Processes*, PFTA, Cracow

11. Szopa R., 2006, *Sensitivity Analysis and Inverse Problems in the Thermal Theory of Foundry Processes*, Publ. of Czest. Univ. of Technology, Częstochowa

Identyfikacja utajonego ciepła krzepnięcia stopów na podstawie wyników analizy termiczno-derywacyjnej

Streszczenie

Analiza termiczno-derywacyjna (ATD) stanowi efektywne narzędzie ilościowej oceny parametrów krzepnięcia stopów odlewniczych (np. temperatury początku i końca krzepnięcia, kinetyki wydzielania się ciepła przemiany, itd.). Urządzenie ATD daje możliwość obserwacji krzywych stygnięcia (nagrzewania) oraz szybkości tych procesów, czyli można również obserwować zmiany pochodnej temperatury względem czasu ($\partial T/\partial t$). W niniejszej pracy rozpatruje się zadanie dotyczące identyfikacji utajonego ciepła krzepnięcia stopów na podstawie informacji wynikających z pomiarów realizowanych urządzeniem ATD. Na etapie obliczeń numerycznych wykorzystano metodę różnic skończonych dla nieliniowych zadań nieustalonego przewodzenia ciepła. W końcowej części pracy przedstawiono wyniki identyfikacji utajonego ciepła krzepnięcia staliwa.

Manuscript received November 17, 2010; accepted for print December 16, 2010