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Algorithms of optimum location of sensors for solidification parameters estimation

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Abstract

The algorithms of optimal sensor location for estimation of solidification parameters are discussed. These algorithms base on the Fisher Information Matrix and A-optimality or D-optimality criterion. Numerical examples of planning algorithms are presented and next for optimal position of sensors the inverse problems connected with the identification of unknown parameters are solved. The examples presented concern the simultaneous estimation of mould thermophysical parameters (volumetric specific heat and thermal conductivity) and also the components of volumetric latent heat of cast iron.

Keywords: Application of information technology to the foundry industry, Solidification process, Numerical techniques, Identification methods, Optimal sensors location

1. Introduction

A fundamental problem connected with the identification of solidification parameters is the selection of sensors location. On the one hand, the limited number of measurement points in the domain considered should be taken into account, on the other hand, the best estimators of solidification parameters are expected. Usually, the location of sensors is dictated by physical conditions and by intuition.

The other approach consists in the application of efficient numerical algorithms of optimum experimental design. The main idea of these algorithms is to define a design criterion basing on the Fisher Information Matrix (FIM) [1] in order to maximize the expected accuracy of the parameter estimates. In literature different optimal criteria exist [1, 2, 3]. The most popular are the A-optimality and D-optimality criterions. In this paper both of them are applied in numerical algorithms assuring the best position of sensors location. The planning algorithms are verified by numerical examples concerning a two-dimensional solidification problem. The examples of inverse problems solution are also shown.

2. Design plan of sensors location

For simplicity it is assumed that two parameters p_1 , p_2 appearing in mathematical model of solidification problem are unknown for example the thermal conductivity and volumetric specific heat of mould. These parameters can be estimated using temperature measurements at the points x^i , $i = 1, 2, \dots , N$ from casting or mould sub-domain

$$T^f_{d\,i} = T_d \; x^i, t^f \;, \qquad f = 1, 2, \dots, F \tag{1}$$

where $t^f = f\Delta t$ and Δt is the time step.

A fundamental problem is the selection of sensors location. The additional problem is connected with determination of sufficient sensors number. It should be pointed out that the number of sensors should be greater or equal to the number of identified parameters (here: $N \geq 2$).

Majority of the methods assuring the best localization of sensors (thermocouples) bases on the Fisher Information Matrix

[1]. To construct this matrix the sensitivity coefficients should be determined, this means

$$Z_{i1}^{f}=\frac{\partial T\left(x^{i},\, t^{f},\, p_{1}^{0},\, p_{2}^{0}\right)}{\partial p_{1}^{0}} \tag{2}$$

and

$$Z_{i2}^{f}=\frac{\partial T\left(x^{i},\, t^{f},\, p_{1}^{0},\, p_{2}^{0}\right)}{\partial p_{2}^{0}} \tag{3}$$

where p_1^0, p_2^0 are the *a priori* estimates of the parameters p_1 , p_2 available e.g. from preliminary experiments.
The following matrix is constructed

$$\mathbf{Z}(x^{i})=\begin{bmatrix} Z_{i1}^{1} & Z_{i2}^{1} \\ Z_{i1}^{2} & Z_{i2}^{2} \\ \ldots & \ldots \\ Z_{i1}^{F} & Z_{i2}^{F} \end{bmatrix} \tag{4}$$

It is easy to check that the product of transpose of a matrix $\mathbf{Z}^{\mathrm{T}}(x^i)$ and matrix $\mathbf{Z}(x^i)$ equals to

$$\mathbf{Z}^{\mathrm{T}}\left(x^{i}\right)\mathbf{Z}\left(x^{i}\right)=\begin{bmatrix} \sum_{f=1}^{F}\left(Z_{i1}^{f}\right)^{2} & \sum_{f=1}^{F} Z_{i1}^{f} Z_{i2}^{f} \\ \sum_{f=1}^{F} Z_{i1}^{f} Z_{i2}^{f} & \sum_{f=1}^{F}\left(Z_{i2}^{f}\right)^{2} \end{bmatrix} \tag{5}$$

The Fisher Information Matrix is as follows [1, 3]

$$\mathbf{M}\left(w_{1}, w_{2}, \ldots, w_{M}\right)=\sum_{i=1}^{M} w_{i}\, \mathbf{Z}^{\mathrm{T}}\left(x^{i}\right) \mathbf{Z}\left(x^{i}\right) \tag{6}$$

where w_1 , w_2 , … , w_M are the weights connected with the points x^i, additionally $0 \le w_i \le 1$, $i = 1, 2, \ldots, M$ and

$$\sum_{i=1}^{M} w_{i}=1 \tag{7}$$

After the mathematical manipulations the FIM takes a form

$$\mathbf{M}\left(w_{1}, \ldots, w_{M}\right)=\begin{bmatrix} \sum_{i=1}^{M} w_{i} \sum_{f=1}^{F}\left(Z_{i1}^{f}\right)^{2} & \sum_{i=1}^{M} w_{i} \sum_{f=1}^{F} Z_{i1}^{f} Z_{i2}^{f} \\ \sum_{i=1}^{M} w_{i} \sum_{f=1}^{F} Z_{i1}^{f} Z_{i2}^{f} & \sum_{i=1}^{M} w_{i} \sum_{f=1}^{F}\left(Z_{i2}^{f}\right)^{2} \end{bmatrix} \tag{8}$$

Different criteria of optimality can be taken into account [1, 2, 3]. One of them is the A-optimality which is connected with the minimization of *trace* of information matrix (6). The other is the D-optimality criterion depending on the maximization of the *determinant* of the information matrix (6).

Using A-optimality criterion the following problem should be solved

$$\begin{aligned} & S\left(w_{1}, w_{2}, \ldots, w_{M}\right)=\operatorname{trace} \mathbf{M}^{-1}\left(w_{1}, w_{2}, \ldots, w_{M}\right) \rightarrow \min \\ & 0 \le w_{i} \le 1, \quad i=1,2, \ldots, M \\ & \sum_{i=1}^{M} w_{i}=1 \end{aligned} \tag{9}$$

If the D-optimality criterion is applied, then problem has the form

$$\begin{aligned} & S\left(w_{1}, w_{2}, \ldots, w_{M}\right)=\operatorname{det} \mathbf{M}\left(w_{1}, w_{2}, \ldots, w_{M}\right) \rightarrow \max \\ & 0 \le w_{i} \le 1, \quad i=1,2, \ldots, M \\ & \sum_{i=1}^{M} w_{i}=1 \end{aligned} \tag{10}$$

So, if we have a set of points $X = \{ x^1 , x^2 , \ldots , x^M \}$ at which measurements may be taken, the practical design problem consists in selecting of corresponding weights w_1 , w_2 , … , w_M which define the best experimental conditions.

It should be pointed out that in the design of optimal sensors location an effective procedure for the computation of sensitivity coefficients should be used. In this work the direct differentiation method has been applied [4, 5, 6, 7] (c.f. chapter 4).

3. Model of solidification process

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

$$x \in \Omega: \quad C(T) \frac{\partial T(x, t)}{\partial t}=\lambda \nabla^{2} T\left(x, t\right) \tag{11}$$

where $C(T)$ is the substitute thermal capacity of alloy, λ is the thermal conductivity, T, x, t denote the temperature, geometrical co-ordinates and time.

The equation (11) is supplemented by the equation concerning a mould sub-domain

$$x \in \Omega_{m}: \quad c_{m} \frac{\partial T_{m}(x, t)}{\partial t}=\lambda_{m} \nabla^{2} T_{m}\left(x, t\right) \tag{12}$$

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

$$x \in \Gamma_{c}: \begin{cases} -\lambda(T)\, \mathbf{n} \cdot \nabla T(x, t)=-\lambda_{m}\, \mathbf{n} \cdot \nabla T_{m}(x, t) \\ T(x, t)=T_{m}(x, t) \end{cases} \tag{13}$$

can be accepted.

On the external surface of the system the Robin condition

$$x\in\Gamma_0: \quad -\lambda_m\,\mathbf{n}\cdot\nabla T_m(x,\,t)=\alpha\;\; T_m(x,\,t)-T_a \tag{14}$$

is given (α is the heat transfer coefficient, T_a is the ambient temperature).
For time t = 0 the initial condition

$$t=0: \quad T(x,\,0)=T_0(x)\;\;,\;\; T_m(x,\,0)=T_{m\,0}(x) \tag{15}$$

is also known.

In the case of cast iron solidification the following approximation of substitute thermal capacity can be taken into account [8, 9, 10]

$$C\;\;T\;\;=\begin{cases} c_L\,, & T>T_L \\ \dfrac{c_L+c_S}{2}+\dfrac{Q_{aus}}{T_L-T_E}\,, & T_E<T\le T_L \\ \dfrac{c_L+c_S}{2}+\dfrac{Q_{eu}}{T_E-T_S}\,, & T_S<T\le T_E \\ c_S\,, & T\le T_S \end{cases} \tag{16}$$

where T_L, T_S are the liquidus and solidus temperatures, respectively, T_E is the temperature corresponding to the beginning of eutectic crystallization, Q_{aus}, Q_{eu} are the latent heats connected with the austenite and eutectic phases evolution, c_L, c_S are constant volumetric specific heats of molten metal and solid one, respectively.

It is assumed that two optional parameters appearing in the mathematical model presented above are unknown, for example thermal conductivity and volumetric specific heat of mould.

4. Sensitivity coefficients

To determine the sensitivity functions the governing equations (11) – (15) are differentiated with respect to parameters p_1 and p_2, respectively. So the differentiation of equations (11), (12) with respect to p_e, e = 1, 2 gives the following formulas
– for casting sub-domain

$$\begin{aligned} x\in\Omega:\;\; &\frac{\partial C(T)}{\partial p_e}\frac{\partial T(x,\,t)}{\partial t}+C(T)\frac{\partial}{\partial p_e}\left(\frac{\partial T(x,\,t)}{\partial t}\right)= \\ &\frac{\partial\lambda}{\partial p_e}\nabla^2 T(x,\,t)+\lambda\frac{\partial}{\partial p_e}\left[\nabla^2 T(x,\,t)\right] \end{aligned} \tag{17}$$

– for mould sub-domain

$$\begin{aligned} x\in\Omega_m:\;\; &\frac{\partial c_m}{\partial p_e}\frac{\partial T_m(x,\,t)}{\partial t}+c_m\frac{\partial}{\partial p_e}\left(\frac{\partial T_m(x,\,t)}{\partial t}\right)= \\ &\frac{\partial\lambda_m}{\partial p_e}\nabla^2 T_m(x,\,t)+\lambda_m\frac{\partial}{\partial p_e}\left[\nabla^2 T_m(x,\,t)\right] \end{aligned} \tag{18}$$

The boundary conditions after differentiation take a form

$$x\in\Gamma_c:\begin{cases} -\dfrac{\partial\lambda}{\partial p_e}\mathbf{n}\cdot\nabla T(x,\,t)-\lambda\dfrac{\partial}{\partial p_e}\;\;\mathbf{n}\cdot\nabla T(x,\,t)\;\;= \\ -\dfrac{\partial\lambda_m}{\partial p_e}\mathbf{n}\cdot\nabla T_m(x,\,t)-\lambda_m\dfrac{\partial}{\partial p_e}\;\;\mathbf{n}\cdot\nabla T_m(x,\,t) \\ \qquad\dfrac{\partial T(x,\,t)}{\partial p_e}=\dfrac{\partial T_m(x,\,t)}{\partial p_e} \end{cases} \tag{19}$$

and

$$\begin{aligned} x\in\Gamma_0:\; &-\frac{\partial\lambda_m}{\partial p_e}\mathbf{n}\cdot\nabla T_m(x,\,t)-\lambda_m\frac{\partial}{\partial p_e}\;\;\mathbf{n}\cdot\nabla T_m(x,\,t)\;\;= \\ &\frac{\partial\alpha}{\partial p_e}\;\;T_m(x,\,t)-T_a\;\;+\alpha\left[\frac{\partial T_m(x,\,t)}{\partial p_e}-\frac{\partial T_a}{\partial p_e}\right] \end{aligned} \tag{20}$$

The initial condition is following

$$t=0:\quad \frac{\partial T(x,\,0)}{\partial p_e}=0\;\;,\;\;\frac{\partial T_m(x,\,0)}{\partial p_e}=0 \tag{21}$$

Introducing the notation

$$Z_e(x,\,t)=\frac{\partial T(x,\,t)}{\partial p_e}\;,\quad Z_{m\,e}(x,\,t)=\frac{\partial T_m(x,\,t)}{\partial p_e} \tag{22}$$

one has

$$\begin{aligned} &x\in\Omega: C(T)\frac{\partial Z_e(x,\,t)}{\partial t}=\lambda\nabla^2 Z_e(x,\,t)+ \\ &\qquad\frac{\partial\lambda}{\partial p_e}\nabla^2 T(x,\,t)-\frac{\partial C(T)}{\partial p_e}\frac{\partial T(x,\,t)}{\partial t} \\ &x\in\Omega_m:\; c_m\frac{\partial Z_{m\,e}(x,\,t)}{\partial t}=\lambda_m\nabla^2 Z_{m\,e}(x,\,t)+ \\ &\qquad\frac{\partial\lambda_m}{\partial p_e}\nabla^2 T_m(x,\,t)-\frac{\partial c_m}{\partial p_e}\frac{\partial T_m(x,\,t)}{\partial t} \\ &x\in\Gamma_c:\begin{cases} -\lambda\mathbf{n}\cdot\nabla Z_e(x,\,t)=-\lambda_m\mathbf{n}\cdot\nabla Z_{m\,e}(x,\,t)- \\ \dfrac{\partial\lambda_m}{\partial p_e}\mathbf{n}\cdot T_{me}(x,\,t)+\dfrac{\partial\lambda}{\partial p_e}\mathbf{n}\cdot\nabla T(x,\,t) \\ \qquad Z_e(x,\,t)=Z_{m\,e}(x,\,t) \end{cases} \\ &x\in\Gamma_0:\; -\mathbf{n}\cdot\nabla T_{me}(x,\,t)-\lambda_m\mathbf{n}\cdot\nabla Z_{m\,e}(x,\,t)= \\ &\qquad\alpha\left[Z_{m\,e}(x,\,t)-\frac{\partial T_a}{\partial p_e}\right] \\ &t=0:\quad Z_e(x,\,0)=0\;\;,\;\; Z_{m\,e}(x,\,0)=0 \end{aligned} \tag{23}$$

5. Algorithm for constructing D-optimal design

The 2D problem is considered as shown in Figure 1. Let $X = \{x^1 = (x_1^1, x_2^1), x^2 = (x_1^2, x_2^2), ..., x^M = (x_1^M, x_2^M)\}$ is the set of points from the casting-mould domain which are taken into account as the possible sensors location (Figure 2).

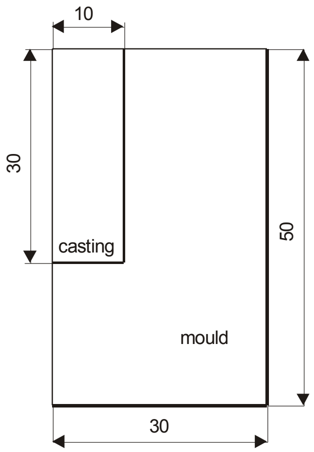

Fig. 1. Casting-mould system

The proposed numerical algorithm consists in the selection of the best positions of sensors under the assumption that only two sensors will be taken into account (it corresponds to the number of estimated parameters). These two sensors we denote by x^i and x^j, respectively.

So, we have

$$\binom{M}{2} \tag{24}$$

possibilities which should be taken into account (it is the combination without repetition, of course). For each pair (x^i, x^j) the following matrix is constructed (c.f. equation (8))

$$\mathbf{M}\left(x^i, x^j\right) = \begin{bmatrix} \sum_{f=1}^{F}\left[\left(Z_{i1}^f\right)^2 + \left(Z_{j1}^f\right)^2\right] & \sum_{f=1}^{F}\left(Z_{i1}^f Z_{i2}^f + Z_{j1}^f Z_{j2}^f\right) \\ \sum_{f=1}^{F}\left(Z_{i1}^f Z_{i2}^f + Z_{j1}^f Z_{j2}^f\right) & \sum_{f=1}^{F}\left[\left(Z_{i2}^f\right)^2 + \left(Z_{j2}^f\right)^2\right] \end{bmatrix} \tag{25}$$

It is the Fisher Information Matrix for two points (c.f. equation (7)) but the weights are here omitted.

D-optimality criterion used in the design of sensors location is the following [11, 12]

$$\det \mathbf{M}\left(x^{i*}, x^{j*}\right) = \max_{(x^i, x^j)} \det \mathbf{M}\left(x^i, x^j\right) \tag{26}$$

The points x^{i*}, x^{j*} correspond to the best position of two sensors.

The algorithm is very simple but time-consuming, because a big number of sensitivity problems should be solved (c.f. formula (25)).

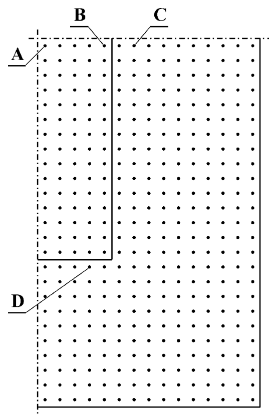

Fig. 2. Possible sensors locations

6. Solution of inverse problem

To solve the inverse problem the least squares criterion is applied

$$S\left(p_1, p_2\right) = \frac{1}{2F}\sum_{i=1}^{M}\sum_{f=1}^{F}\left(T_i^f - T_{di}^f\right)^2 \tag{27}$$

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 of the parameters p_1 , p_2 e.g. from preliminary experiments.

In the case of typical gradient method application [8, 9, 10, 13, 14, 15] the criterion (27) is differentiated with respect to the unknown parameters p_e , $e = 1, 2$ and next the necessary condition of optimum is used. Finally one obtains the following system of equations

$$\frac{\partial S}{\partial p_e} = \frac{2}{MF}\sum_{i=1}^{M}\sum_{f=1}^{F}\left(T_i^f - T_{di}^f\right)\left(Z_{ie}^f\right)^k = 0\ ,\ e = 1, 2 \tag{28}$$

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

$$T_i^f = \left(T_i^f\right)^k + \sum_{l=1}^{2}\left(Z_{il}^f\right)^k\left(p_l^{k+1} - p_l^k\right) \tag{29}$$

Introducing (29) into (28) one obtains ($e = 1, 2$)

$$\sum_{i=1}^{M}\sum_{f=1}^{F}\sum_{l=1}^{2} \left(Z_{il}^{f}\right)^{k} \left(Z_{ie}^{f}\right)^{k} \left(p_{l}^{k+1}-p_{l}^{k}\right) =$$

$$\sum_{i=1}^{M}\sum_{f=1}^{F}\left[T_{di}^{f}-\left(T_{i}^{f}\right)^{k}\right]\left(Z_{ie}^{f}\right)^{k} \qquad (30)$$

The system of equations (30) can be written in the matrix form

$$\left(\mathbf{Z}^{k}\right)^{\mathrm{T}}\mathbf{Z}^{k}\left(\mathbf{p}^{k+1}-\mathbf{p}^{k}\right) = \left(\mathbf{Z}^{k}\right)^{\mathrm{T}}\left(\mathbf{T}_{d}-\mathbf{T}^{k}\right) \qquad (31)$$

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

7. Examples of computations

To solve the system of equations (11)-(15) and additional problems (23) connected with the sensitivity functions the explicit scheme of the finite difference method (FDM) for non-linear parabolic equations [16] is applied.

For direct problem in which all solidification parameters are known the following input data have been introduced: λ = 30 [W/(mK)],
c_L = 5.88 [MJ/(m^3 K)], c_S = 5.4 [MJ/(m^3 K)], Q_{aus}= 923 [MJ/m^3], Q_{eu} = 994 [MJ/m^3], λ_m =1 [W/(mK)], c_m =1.75 [MJ/(m^3 K)], pouring temperature T_0 = 1300^{o}C, liquidus temperature T_L = 1250^{o}C, border temperature T_E =1160^{o}C, solidus temperature T_S = 1110^{o}C, initial mould temperature T_{m0} = 20^{o}C.

The regular mesh created by 25×15 nodes with constant step h = 0.002 [m] (Figure 2) has been introduced, time step Δt = 0.1 [s]. It is assumed that the possible co-ordinates of sensors correspond to the co-ordinates of FDM nodes, because the values of sensitivities for this set of points are directly known.

The proposed algorithm of optimal sensors location (c.f. Chapter 6) can be used under the assumption that number of sensors equals 2. Using this algorithm two identification problems are solved.

The first problem concerns the simultaneous identification of austenite latent heat $p_1 = Q_{aus}$ and eutectic latent heat $p_2 = Q_{eu}$ [11].

The problem of optimal sensors location has been solved under the assumption that Q_{aus}^0 = 900 [MJ/m^3], $Q_{eu}^{\,0}$ = 1000 [MJ/m^3] and the possible sensors are located in the casting sub-domain. The application of optimization procedure shows that the best sensors position corresponds to the nodes from casting domain marked by A and B in Figure 2.

In Figure 3 the cooling curves at the points A and B are shown. The results of identification are presented in Figure 4. It is visible, that the iteration process is convergent and the number of iterations is very small.

The second inverse problem is connected with the simultaneous identification of mould parameters, this means thermal conductivity λ_m and volumetric specific heat c_m.

The problem of optimal sensors location has been solved under the assumption that λ_m^0 = 0.5 [W/(mK)], c_m^0 = 1 [MJ/(m^3 K)] and possible sensors are from the mould sub-domain. The best sensors position corresponds to the nodes marked by C and D in Figure 2.

In Figure 5 the heating curves at the points C and D are shown. The results of identification are presented in Figure 5. As previously, it is visible, that the iteration process is convergent and the number of iterations is very small.

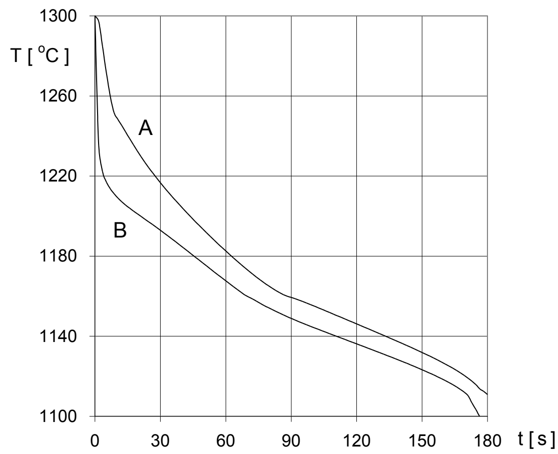

Fig. 3. Cooling curves

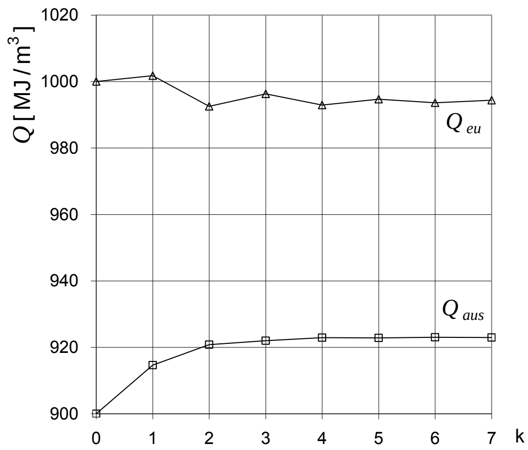

Fig. 4. Inverse problem solution (Q_{aus}, Q_{eu})

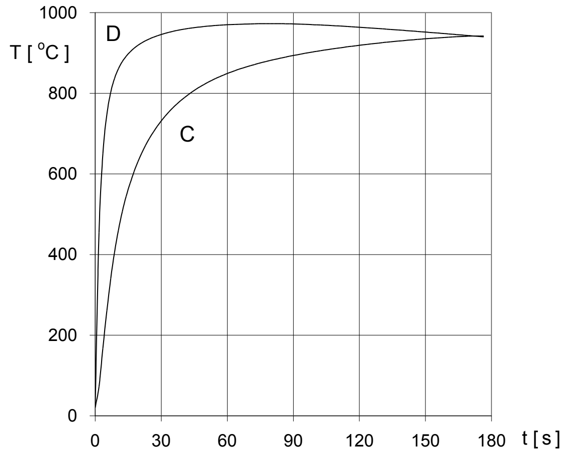

Fig. 5. Heating curves

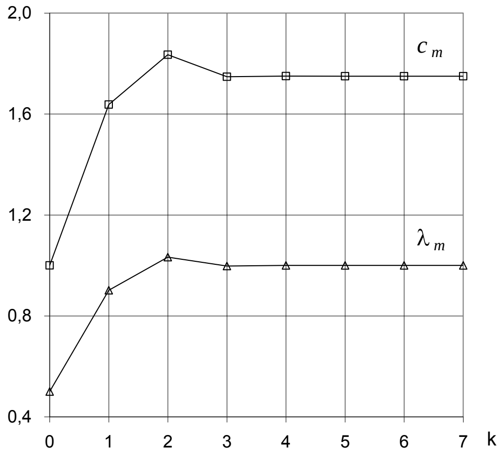

Fig. 6. Inverse problem solution (c_m, λ_m)

8. Conclusions

The problem of optimum location of sensors for simultaneous estimation of two solidification parameters has been discussed. Known from the literature the A-optimality and D-optimality criterions have been extended on the non-steady state problems. The algorithm of D-optimal design basing on the modified for non-steady problems Fisher Information Matrix has been proposed. Using this algorithm two examples have been solved.

For the optimal sensors location the inverse problems solutions have been found by means of the gradient method. The effectiveness of this method is connected with the proper choice of starting point and the convergence of iteration process. One can see the good properties of inverse problem solution in the case of „the best" position of sensors (Figures 4 and 6). Additionally, the number of iterations necessary in order to obtain the final results is very small.

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