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ESTIMATION OF SOURCE TERM PARAMETERS DURING SOLID-SOLID PHASE TRANSFORMATION OF STEELS

Rafaela Bellini
Department of Mechanical and Aerospace Engineering
The University of Texas at Arlington
Arlington, TX, USA

Helcio R. B. Orlande
Department of Mechanical Engineering, POLI/COPPE
Federal University of Rio de Janeiro, UFRJ
Rio de Janeiro, RJ, Brazil
helcio@serv.com.ufrj.br

Juan Garcia de Blas
Department of Metallurgical and Materials Engineering, POLI/COPPE
Federal University of Rio de Janeiro, UFRJ
Rio de Janeiro, RJ, Brazil
jgarcia@metalmat.ufrj.br

ABSTRACT

The objective of this work is to estimate the heat-source term associated with pearlitic phase transformation in steels. The transformation rate is assumed to be given in terms of Johnson-Mehl-Avrami's model. As a result, the present inverse heat conduction problem is reduced to the estimation of four parameters appearing in the formulation for this model. The Levenberg-Marquardt method of minimization of the least-squares norm is used for the estimation of the unknown parameters, by using simulated transient temperature measurements taken inside the medium. The D-optimum approach is applied for the design of the experiment with respect to different experimental variables, including the number and locations of sensors, the duration of the experiment and the heat transfer boundary conditions during the cooling of the specimen.

NOMENCLATURE

C volumetric heat capacity
e slab thickness
g heat source term
h_∞ heat transfer coefficient
H enthalpy
I number of transient measurements per sensor
J sensitivity coefficients
$\mathbf{J}$ sensitivity matrix
k thermal conductivity
K function of temperature appearing in Johnson-Mehl-Avrami's model (see eq. (1))
M number of sensors
n function of temperature appearing in Johnson-Mehl-Avrami's model (see eq. (1))
P_j unknown parameters, j=1,...,4
$\mathbf{P}$ vector of unknown parameters
S least-squares norm
T temperature
T_∞ temperature of the cooling fluid and surroundings
t time
$\mathbf{T}$ vector of estimated temperatures
t_f final time
$\mathbf{V}$ covariance matrix
X normalized sensitiviy coefficients
x spatial variable
Y measured temperatures
$\mathbf{Y}$ vector of measured temperatures

Greeks

a transformed fraction
e emissivity
Δ variation
r density
s standard-deviation of the measurements
s_r Steffan-Boltzmann constant

Subscripts

i refers to time t_i, i = 1, …, I
m refers to the sensor number, m = 1, …, M
a refers to austenite
p refers to pearlite

INTRODUCTION

Identification, optimization and control of the thermal conditions in industrial manufacturing processes are of major interest, because of their capital importance in quality control, as well as in the reduction of product damages, energy consumption and production losses. In the steel industry, research in this area generally aims at manufacturing steel products with tight specifications for mechanical resistance and tenacity. One example is the appropriate selection of the cooling techniques to control the steel microstructure resultant from phase transformations, after large deformations at high temperatures.

In this paper, we solve the inverse problem of estimating four parameters appearing in Johnson-Mehl-Avrami's model for the phase transformation rate in pearlitic steels [1-4]. The main objective of the paper is to examine the possibility of using transient temperature measurements of the material in order to estimate the phase transformation rate of steels that follow Johnson-Mehl-Avrami's model for the phase transformation. The use of simple and cheap temperature measurements may avoid the necessity of quite expensive experimental apparatuses to identify the phase transformation rate. Similar works have been performed by Jarny et al [5-10] in the identification and control of vulcanization of rubber and plastics.

For the solution of the present parameter estimation problem we use the Levenberg-Marquardt method of minimization of the least-squares norm [11-14], with simulated temperature measurements. The D-optimum approach is applied for the design of the experiment with respect to different experimental variables, including the number and locations of sensors, the duration of the experiment and the heat transfer boundary conditions during the cooling of the specimen [11,14].

PHYSICAL PROBLEM AND MATHEMATICAL FORMULATION

The physical problem considered here involves the cooling of a one-dimensional *pearlitic steel* slab of thickness $2e$. The slab, initially at the uniform temperature T_0 and in the austenitic phase, is cooled by convection and radiation at both boundaries with identical conditions, involving a constant heat transfer coefficient and a constant emissivity. Solid-solid phase transformations from austenite to pearlite take place in the steel slab as it is cooled. Therefore, the source term resulting from the phase transformation needs to be taken into account in the energy conservation equation. Because of the phase transformation, physical properties depend on the phase fraction. Due to the large temperature variations during the cooling process, the temperature dependence of the physical properties need also to be taken into account.

The phase transformation kinetics can be experimentally determined at different constant temperatures, resulting in the transformation-time-temperature (TTT) diagrams [1-3]. With these diagrams, the development of the isothermal phase transformation can be conveniently represented in terms of the transformed fraction, a, as a function of time and temperature.

Johnson-Mehl-Avrami's model for the isothermal phase transformation can be written in the following general form for the transformed fraction [2]:

$$a = 1 - \exp\left(-K\, t^n\right) \tag{1}$$

By assuming that the instantaneous transformation rate is a function of temperature and of the transformed fraction, that is, the reaction is additive [2], it is possible to determine the non-isothermal transformation history from the isothermal transformation curves. Then, we can write for Johnson-Mehl-Avrami's model:

$$\frac{\partial a}{\partial t} = K^{1/n}\, n\left[\ln\left(\frac{1}{1-a}\right)\right]^{\frac{n-1}{n}}(1-a) \tag{2}$$

By taking into account the symmetry of the physical heat conduction problem examined in this paper, we can write its mathematical formulation as:

$$C(T,a)\frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left[k(T,a)\frac{\partial T}{\partial x}\right] + g(T,a)$$

in $0 < x < e$, for $t > 0$ (3.a)

$$k(T,a)\frac{\partial T}{\partial x} = 0 \quad \text{at } x = 0, \text{ for } t > 0 \tag{3.b}$$

$$k(T,a)\frac{\partial T}{\partial x} + h_\infty T + e\, s_r\, T^4 = h_\infty T_\infty + e\, s_r\, T_\infty^4$$

at $x = e$, for $t > 0$ (3.c)

$$T = T_0 \quad \text{for } t = 0, \text{ in } 0 < x < e \tag{3.d}$$

where the source term resulting from the phase transformation is given by

$$g(T,a) = r\,\Delta H(T)\frac{\partial a(T,a)}{\partial t} \tag{4.a}$$

with the initial condition

$$a = 0 \quad \text{for } t = 0, \text{ in } 0 < x < e \tag{4.b}$$

The transformed fraction, a, is computed in this work with Johnson-Mehl-Avrami's model given by equation (1). For a *pearlitic AFNOR XC70 steel* (equivalent to ASTM-1080), the following approximations can be used for K and n, respectively, appearing in such a model [3]:

$$\hat{E} = \left(\frac{41210}{T} - 49.679 \right) \tag{5.a}$$

$$n = 12.904 - 0.012T \tag{5.b}$$

For this type of pearlitic steel, the enthalpy change during phase-change is given by [4]:

$$\Delta H(T) = -37427 + 421.689\,T + 0.37997\,T^2 \quad \left[\mathrm{J}/\mathrm{kg} \right] \tag{6.a}$$

while the thermal conductivities and specific heats of the austenitic and pearlitic phases are given respectively by [4]:

$$k_a(T) = 7.522104 + 0.0152214\,T \quad \left[W/m\ K \right] \tag{6.b}$$

$$k_p(T) = 55.593227 - 0.0260404T \quad \left[W/m\ K \right] \tag{6.c}$$

$$c_a(T) = 422.31 + 0.150T \quad \left[\mathrm{J}/\mathrm{kg\,K} \right] \tag{6.d}$$

$$c_p(T) = 0.621 - 0.91T \quad \left[\mathrm{J}/\mathrm{kg\,K} \right] \tag{6.e}$$

The volumetric heat capacity and the thermal conductivity of the slab, as a function of temperature and of the transformed fraction, are obtained by using equations (6.b-e) and a volumetric averaging as follows:

$$C(T, a) = r[a\,c_p(T) + (1-a)c_a(T)] \tag{7.a}$$

$$k(T, a) = a\ k_p(T) + (1-a)k_a(T) \tag{7.b}$$

where r = 7600 kg/m^3.

DIRECT AND INVERSE PROBLEMS

In the *direct problem* associated with the mathematical formulation of the physical problems described above, boundary and initial conditions, as well as the thermophysical properties and the source-term resulting from the phase transformation, are known. The objective of the direct problem is to determine the transient temperature field in the slab.

On the other hand, associated with such mathematical formulation we can also envision the *inverse problem* of interest here, which is concerned with the identification of the phase transformation rate. In order to identify such quantity, we assume available temperature measurements taken inside the slab. For the solution of the inverse problem, we also assume that the boundary and initial conditions for the slab, as well as the thermophysical properties given by equations (6.a-e, 7.a,b), are known with high degree of accuracy. The temperature measurements contain errors, which are assumed to be additive, uncorrelated, normally distributed, with zero mean and constant and known standard-deviation [11].

For the solution of the inverse problem, we assume *a priori* that the transformed fraction is given in terms of Johnson-Mehl-Avrami's model. The temperature-dependent functions K and n appearing in equation (1) are assumed to be given by the following expressions, analogous to equations (5.a,b):

$$K = \exp\left(\frac{P_1}{T} - P_2 \right) \qquad n = (P_3 - P_4\,T) \tag{8.a,b}$$

Therefore, the inverse problem of estimating the phase transformation rate is reduced to the estimation of the 4 unknown parameters P_j, j = 1, 2, 3 and 4 appearing in equations (8.a,b). These four parameters are estimated with the minimization of the least-squares norm.

SOLUTION OF THE INVERSE PROBLEM

The minimization of the least-squares norm result in a minimum variance estimator with the hypotheses described above for the measurement errors [11]. The least squares norm is written in vector form as

$$S(\mathbf{P}) = [\mathbf{Y} - \mathbf{T}(\mathbf{P})]^T [\mathbf{Y} - \mathbf{T}(\mathbf{P})] \tag{9}$$

where the superscript T denotes the vector transpose and

$$[\mathbf{Y} - \mathbf{T}(\mathbf{P})]^T = [\vec{Y}_1 - \vec{T}_1(\mathbf{P}), \vec{Y}_2 - \vec{T}_2(\mathbf{P}), \cdots, \vec{Y}_I - \vec{T}_I(\mathbf{P})] \tag{10.a}$$

The element $[\vec{Y}_i - \vec{T}_i(\mathbf{P})]$ is a vector containing the difference between the measured and the estimated temperatures for the M sensors at time t_i, that is,

$$[\vec{Y}_i - \vec{T}_i(\mathbf{P})] = [Y_{i1} - T_{i1}(\mathbf{P}), Y_{i2} - T_{i2}(\mathbf{P}), \cdots, Y_{iM} - T_{iM}(\mathbf{P})] \quad \text{for } i = 1, \ldots, I \tag{10.b}$$

For the minimization of the least squares norm (9), we apply the *Levenberg-Marquardt Method* [11-14]. The iterative procedure of such a method is given by:

$$\mathbf{P}^{k+1} = \mathbf{P}^k + [(\mathbf{J}^k)^T \mathbf{J}^k + m^k \mathbf{\Omega}^k]^{-1} (\mathbf{J}^k)^T [\mathbf{Y} - \mathbf{T}(\mathbf{P}^k)] \tag{11}$$

where μ^k is a positive scalar named *damping parameter*, $\mathbf{\Omega}^k$ is a *diagonal matrix* and $\mathbf{J}^k$ is the *sensitivity matrix*. The sensitivity matrix is defined as

$$\mathbf{J}(\mathbf{P}^k) = \left[\frac{\partial \mathbf{T}^T(\mathbf{P})}{\partial \mathbf{P}} \right]^T \qquad (12)$$

STATISTICAL ANALYSIS

By performing a statistical analysis it is possible to assess the accuracy of $\hat{P}_j$, j = 1, 2, 3 and 4, which are the values estimated for the unknown parameters P_j, 1, 2, 3 and 4. By taking into account the statistical hypotheses described above, the *covariance matrix* for the ordinary least-squares estimator is given by [11]:

$$\mathbf{V} = (\mathbf{J}^T\mathbf{J})^{-1} s^2 \qquad (13)$$

where s is the standard deviation of the measurement errors, which is assumed to be constant. We note that equation (13) is exact for linear estimation problems and is approximately used for nonlinear parameter estimation problems.

The *standard deviations* for the estimated parameters can thus be obtained from the diagonal elements of **V** as

$$s_j = \sqrt{V_{jj}} \quad \text{for } j = 1, 2, 3 \text{ and } 4 \qquad (14)$$

where V_{jj} is the j^{th} element in the diagonal of **V**.

Confidence intervals at the 99% confidence level for the estimated parameters can be obtained as

$$\hat{P}_j - 2.576 s_j \le P_j \le \hat{P}_j + 2.576 s_j$$
$$\text{for } j = 1, 2, 3 \text{ and } 4 \qquad (15)$$

The *joint confidence region* for the estimated parameters is given by [11]:

$$(\hat{\mathbf{P}} - \mathbf{P})^T \mathbf{V}^{-1} (\hat{\mathbf{P}} - \mathbf{P}) \le c_4^2 \qquad (16)$$

where c_4^2 is the value of the chi-square distribution with 4 degrees of freedom for a given probability.

DESIGN OF OPTIMUM EXPERIMENTS

Optimum experiments can be designed by minimizing the hypervolume of the confidence region of the estimated parameters, in order to ensure minimum variance for the estimates. The minimization of the confidence region given by equation (16) can be obtained by maximizing the determinant of $\mathbf{V}^{-1}$, in the so-called *D-optimum design* [11,14]. Since the covariance matrix **V** is given by equation (13), we can then design optimum experiments by maximizing the determinant of the so-called Fisher's Information Matrix, $\mathbf{J}^T\mathbf{J}$ [11,14]. Therefore, optimal experimental variables are chosen based on the criterion

$$\max \left| \mathbf{J}^T \mathbf{J} \right| \qquad (17)$$

For cases involving a single sensor, each element $\mathbf{F}_{r,s}$, r,s = 1, 2, 3 and 4, of the matrix $\mathbf{F} \equiv \mathbf{J}^T\mathbf{J}$ is given by:

$$\mathbf{F}_{r,s} \equiv [\mathbf{J}^T\mathbf{J}]_{r,s} = \sum_{i=1}^{I} \left(\frac{¶ T_i}{¶ P_r} \right) \left(\frac{¶ T_i}{¶ P_s} \right)$$
$$\text{for } r,s = 1, 2, 3 \text{ and } 4 \qquad (18)$$

where I is the number of measurements.

If we take into account constraints, such as a large but fixed number of transient measurements of M sensors, we can choose to maximize the determinant of a normalized form of **F**, here denoted as $\mathbf{F}_I$ [11], the elements of which are given by:

$$[\mathbf{F}_I]_{r,s} = \frac{1}{M t_f} \sum_{m=1}^{M} \int_{t=0}^{t_f} \left(P_r \frac{¶ T_m}{¶ P_r} \right) \left(P_s \frac{¶ T_m}{¶ P_s} \right) dt$$
$$\text{for } r,s = 1, 2, 3 \text{ and } 4 \qquad (19)$$

where t_f is the duration of the experiment.

RESULTS AND DISCUSSIONS

For the results presented below we assume the steel slab to be initially at the uniform temperature T_0 = 1000 K. The half-thickness of the slab is taken as e = 0.050 m and the surface emissivity as e = 0.21. The effects of the heat transfer coefficient on the solution of the inverse problem are examined below.

The direct problem was solved by finite-differences with implicit discretization. An iterative method was required because of the strong non-linear character of the problem, resultant from the temperature and phase dependent properties and from the radiation boundary condition at $x = e$. For the integration of the phase fraction in time a fifth-order Runge-Kutta method was utilized.

We note that for nonlinear estimation problems, such as the one under picture in this work, the analyses of the sensitivity coefficients and of the determinant of $\mathbf{F}_I$ are not global, because these quantities are functions of the unknown parameters. Therefore, *a priori* estimated values for the parameters are required for the design of optimum experiments. For the test-cases examined in this paper, we used the following value for the parameters, based on the data for the pearlitic 1080 steel (see equations

5.a,b): P_1 = 41210, P_2 = 49.679, P_3 = =12.904 and P_4 = 0.012.

Figures 1.a,b present the temperature and the transformation fraction variations, respectively, at selected positions in the medium, for $h_\infty = 10\ \text{W/m}^2\text{K}$. We note in figure 1.b that, for such value of the heat transfer coefficient, the phase transformation is not complete in the slab until 300 s. Figures 2.a,b present analogous results to those presented in figures 1.a,b, but for $h_\infty = 1000\ \text{W/m}^2\text{K}$. Differently than for $h_\infty = 10\ \text{W/m}^2\text{K}$ (see figures 1.a,b), the results presented in figures 2.a,b show that the phase transformation in the slab is complete around 180 s. The effects of the phase transformation on the temperature field is more noticeable for the larger value of the heat transfer coefficient. As compared to a case without phase transformation (energy-source set to zero), the effects of the phase transformation are to increase the temperature level in the slab and to reduce the cooling rate. In fact, an increase in the cooling rate is noticed in figure 2.a at x = 0, when the phase transformation finishes around 180 s.

Figures 3.a,b present the normalized sensitivity coefficients with respect to the different parameters, for x = 0 and x = e, respectively, for $h_\infty = 10\ \text{W/m}^2\text{K}$. The normalized sensitivity coefficients are given by:

$$X_1 = P_1 \frac{\partial T}{\partial P_1} \quad , \quad X_2 = P_2 \frac{\partial T}{\partial P_2} \quad , \quad X_3 = P_3 \frac{\partial T}{\partial P_3}, \quad X_4 = P_4 \frac{\partial T}{\partial P_4} \tag{20.a-d}$$

Figures 3.a,b show that the sensitivity coefficients are relatively large at both positions x = 0 and x = e and, hence, the temperature measurements are very sensitive to perturbations in the unknown parameters. On the other hand, the sensitivity coefficients are highly linearly dependent on both positions. An examination of figures 3.a.b reveals that, although linearly dependent, the shape of the sensitivity coefficients at x = 0 and at x = e are not the same. Similar qualitative behavior was noticed with the analysis of the sensitivity coefficients for $h_\infty = 1000\ \text{W/m}^2\text{K}$.

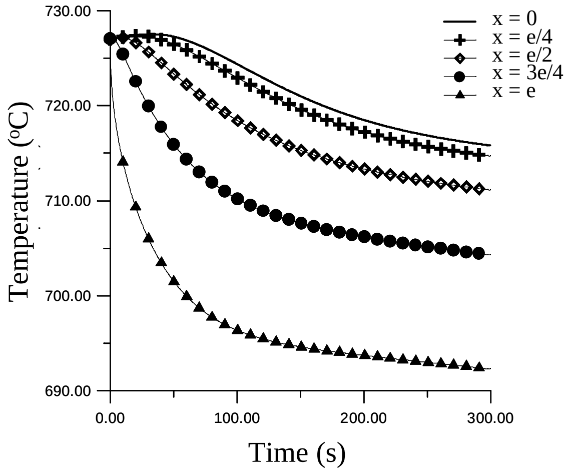

Figure 1.a. Temperature variation in the slab for $h_\infty = 10\ \text{W/m}^2\text{K}$

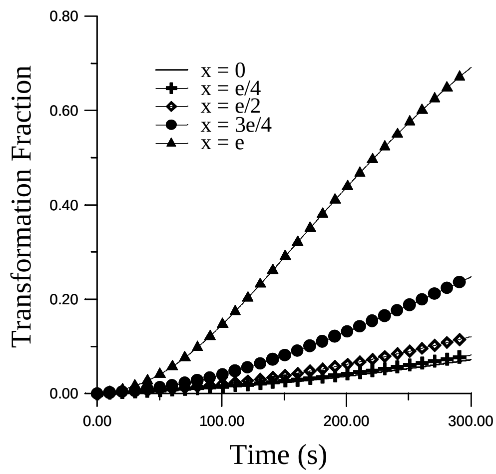

Figure 1.b. Transformation fraction variation in the slab for $h_\infty = 10\ \text{W/m}^2\text{K}$

The transient variation of the determinant of the information matrix, obtained with different numbers of sensors, is presented in figure 4 for $h_\infty = 10\ \text{W/m}^2\text{K}$. The sensor locations are shown in table 1.

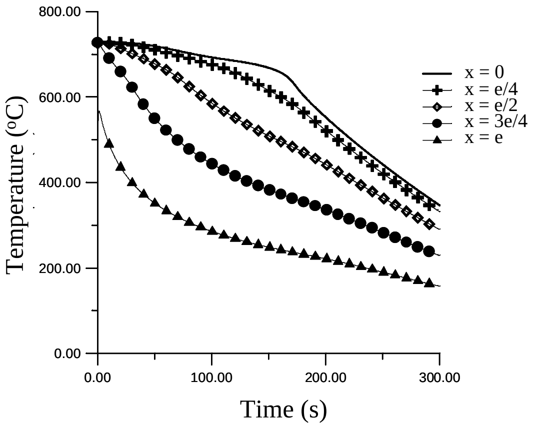

Figure 2.a. Temperature variation in the slab for $h_\infty = 1000$ W/m^{2}K

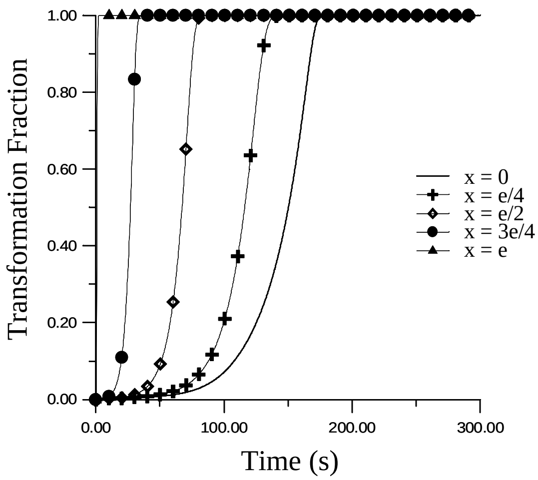

Figure 2.b. Transformation fraction variation in the slab for $h_\infty = 1000$ W/m^{2}K

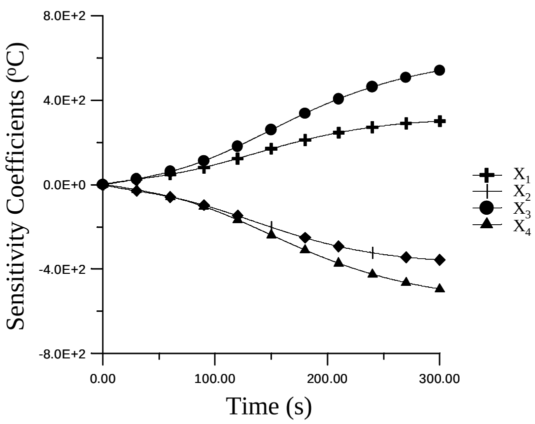

Figure 3.a Sensitivity coefficients at $x = 0$ for $h_\infty = 10$ W/m^{2}K

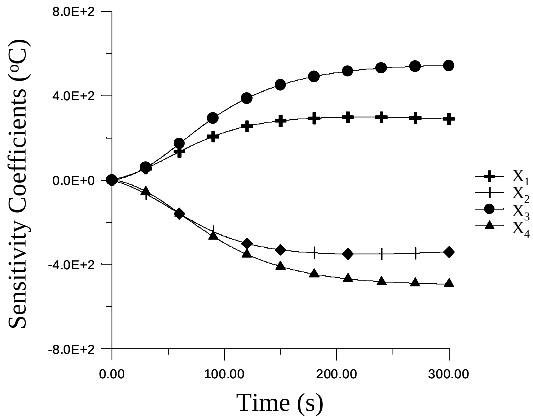

Figure 3.b Sensitivity coefficients at $x = e$ for $h_\infty = 10$ W/m^{2}K

Table 1. Sensor locations

Number of sensors	Sensor Locations
1	$x = e$
2	$x = 0$ and $x = e$
3	$x = 0$, $x = e/2$ and $x = e$
5	$x = 0$, $x = e/4$, $x = e/2$, $x = 3e/4$ and $x = e$

We note in figure 4 that the determinant of the information matrix is null when the measurements of one single sensor are used for the inverse analysis. This is a result of the linear dependency of the sensitivity coefficients, as illustrated in figure 3.b for $x = e$.

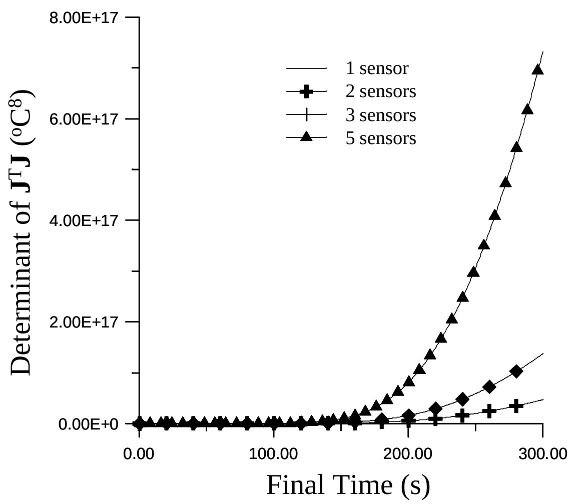

Figure 4. Determinant of the information matrix for $h_\infty = 10$ W/m^{2}K

As the measurements of more sensors are made available, the determinant of the information matrix increases, because the sensitivity coefficients at the different positions have different shapes, although being locally linearly dependent. Such a fact results in columns of the sensitivity matrix linearly independent, reducing the ill-conditioned character of the problem and making possible the estimation of the parameters with more than 1 sensor. The optimum duration of the experiment for $h_\infty = 10\ \mathrm{W/m^2K}$ is larger than 300 s, because the determinant of the information matrix still increases at high rates at 300 s.

Figure 5 illustrates the determinant of the information matrix for $h_\infty = 1000\ \mathrm{W/m^2K}$, for the same measurement positions presented in table 1. We note in figure 5 that, as for $h_\infty = 10\ \mathrm{W/m^2K}$, the determinant is null if one single sensor is used in the analysis because of linearly dependent sensitivity coefficients. Figure 5 shows that the optimum duration of the experiment is around 150 s for the cases with 2 and 3 sensors, and around 130 s for 5 sensors, when the determinant of the information matrix is maximum. A comparison of figures 4 and 5 shows that the maximum values of the determinant for $h_\infty = 1000\ \mathrm{W/m^2K}$ are larger than for $h_\infty = 10\ \mathrm{W/m^2K}$, within the time range examined (up to 300 s). Therefore, for the estimation of the unknown parameters, the experimental conditions should be such that result on large heat transfer coefficients, like those involving boiling of the cooling fluid. The use of large cooling rates can result on accurate estimates for the unknown parameters in a fast experiment, as illustrated below.

Table 2 summarizes the results obtained for the 4 unknown parameters, with the measurements of 3 sensors located in accordance with table 1, for $h_\infty = 10\ \mathrm{W/m^2K}$ and $h_\infty = 1000\ \mathrm{W/m^2K}$. Table 2 presents the estimated parameters as well as their correspondent 99% confidence intervals. The results shown in table 2 were obtained with 200 simulated measurements per sensor, containing random errors of standard deviation 1 K. Based on the analysis of the determinant of the information matrix, the duration of the experiment was taken as 300 s for $h_\infty = 10\ \mathrm{W/m^2K}$ and as 150 s for $h_\infty = 1000\ \mathrm{W/m^2K}$. Initial guesses 50 % larger than the exact parameters were used for the iterative procedure of the Levenberg-Marquardt method of minimization of the least-squares norm. In order to avoid any bias introduced by the random number generator used to compute the simulated measurements, the results presented in table 2 were averaged over 40 runs of the inverse problem solution.

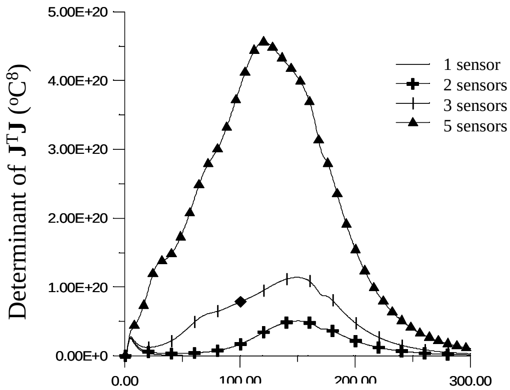

Figure 5. Determinant of the information matrix for $h_\infty = 1000\ \mathrm{W/m^2K}$

Table 2 – Parameters estimated with simulated measurement errors of standard-deviation 1 K

Parameters	$h_\infty = 10\ \mathrm{W/m^2K}$	$h_\infty = 1000\ \mathrm{W/m^2K}$
P_1	45225 ± 43568	42570 ± 2353
P_2	53 ± 44	51 ± 3
P_3	12 ± 8	12 ± 1
P_4	0.011 ± 0.008	0.014 ± 0.001

Table 2 shows that the Levenberg-Marquardt method was able to estimate parameters quite close to the exact ones, for the two values examined for the heat transfer coefficient. On the other hand, as expected from the analysis of the determinant of the information matrix, the confidence intervals obtained with $h_\infty = 1000\ \mathrm{W/m^2K}$ are much smaller than those obtained with $h_\infty = 10\ \mathrm{W/m^2K}$. In fact, quite accurate estimated parameters could be obtained even for a standard-deviation of 2 K, by using $h_\infty = 1000\ \mathrm{W/m^2K}$; but, for such level of measurement error, the Levenberg-Marquardt method did not reach convergence with $h_\infty = 10\ \mathrm{W/m^2K}$.

CONCLUSIONS

The main objective of this paper was to examine the possibility of using transient temperature measurements to estimate the phase-transformation rate of pearlitic steels that follow Johnson-Mehl-Avrami's model for the phase transformation. The unknown transformation rate was parameterized, so that the inverse problem was reduced to the estimation of 4 unknown parameters.

The design of the experimental conditions with the D-optimum approach revealed that accurate estimates can be obtained in fast experiments by using large heat transfer coefficients. Under such experimental conditions, accurate estimates were obtained with the Levenberg-Marquardt method of minimization of the least-squares norm, by using simulated temperature measurements containing random errors.

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