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TRANSIENT HEAT CONDUCTION IN A SOLID CYLINDER WITH CONVECTIVE BOUNDARY CONDITIONS – PART I: INVERSE PROBLEM OF PARAMETER ESTIMATION

H. R. B. Orlande
Department of Mechanical Engineering, POLI/COPPE, Federal University of Rio de Janeiro, UFRJ, Cid Universitaria, Cx. Postal 68503, Rio de Janeiro, RJ, 21945-970, BRAZIL
helcio@serv.com.ufrj.br

A. Haag

F. P. J. de Barros

O. Wellele

P. M. P. da Silva

R. B. Storch

R. de Sá Padilha

Abstract. *This paper presents the solution of an inverse heat transfer problem of parameter estimation. The physical problem considered here involves the heating of a solid cylinder by hot water in a temperature-controlled bath. This paper addresses the identification of unknown parameters appearing in the mathematical formulation of the physical problem, including the cylinder thermal conductivity and volumetric heat capacity, as well as the heat transfer coefficient between the cylinder and water. Temperature measurements taken at selected positions within the cylinder are assumed available for the inverse analysis. Analyses of the sensitivity coefficients with respect to each of the unknown parameters and of the determinant of the information matrix are presented in the paper, for test-cases involving Teflon cylinders of two different sizes and one aluminum cylinder. The unknown parameters are estimated with the Levenberg-Marquardt method of minimization of the least-squares norm. Results obtained with actual experimental measurements are presented in the paper. This work was performed within the scope of a graduate course in the Department of Mechanical Engineering of COPPE/UFRJ. The last six authors of this paper are the students of this course; they are listed in alphabetical order, irrespective of their grade in the course.*

Keywords. *Inverse problems, heat transfer, parameter estimation*

1. Introduction

Inverse heat transfer problems rely on temperature and/or heat flux measurements for the estimation of unknown quantities appearing in the analysis of physical problems in this field. As an example, inverse problems dealing with heat conduction have been generally associated with the estimation of an unknown boundary heat flux, by using temperature measurements taken below the boundary surface. Therefore, while in the classical direct heat conduction problem the cause (boundary heat flux) is given and the effect (temperature field in the body) is determined, the inverse problem involves the estimation of the cause from the knowledge of the effect.

The use of inverse analysis techniques represents a *new research paradigm* (Beck, 1999). The results obtained from numerical simulations and from experiments are not simply compared *a posteriori*, but a close synergism exists between experimental and theoretical researchers during the course of the study, in order to obtain the maximum of information regarding the physical problem under picture.

Inverse problems are mathematically classified as *ill-posed*, whereas standard heat transfer problems are *well-posed* (Hadamard, 1923). The solution of a well-posed problem must satisfy the conditions of existence, uniqueness and stability with respect to the input data. The existence of a solution for an inverse heat transfer problem may be assured by physical reasoning. On the other hand, the uniqueness of the solution of inverse problems can be mathematically proved only for some special cases. Also, the inverse problem is very sensitive to random errors in the measured input data, thus requiring special techniques for its solution in order to satisfy the stability condition (Alifanov, 1994; Alifanov *et al.*, 1995; Beck *et al.*, 1977; Beck *et al.*, 1985; Denisov, 1999; Dulikravich *et al.*, 1996; Hensel, 1991; Kurpisz *et al.*, 1995; Morozov, 1984; Murio, 1993; Ramm *et al.*, 2000; Ozisik *et al.*, 2000; Sabatier, 1978; Tikhonov *et al.*, 1977; Trujillo *et al.*, 1997 and Yagola *et al.*, 1999). A successful solution of an inverse problem generally involves its reformulation as an approximate well-posed problem and makes use of some kind of regularization (stabilization) technique. In several methods, the solution for the inverse problem is obtained in the least-squares sense.

Inverse problems can be solved either as a *parameter estimation* approach or as a *function estimation* approach. If some information is available on the functional form of the unknown quantity, the inverse problem can be reduced to the estimation of few unknown parameters. On the other hand, if no prior information is available on the functional form of the unknown, the inverse problem can be regarded as a *function estimation approach in an infinite dimensional space of functions*.

This paper deals with the solution of a parameter estimation problem involving the heating of a solid cylinder in a temperature-controlled water bath. The inverse problem is concerned with the estimation of the parameters appearing in the mathematical formulation of the physical problem, including the heat transfer coefficient between the body surfaces and the water, as well as the thermal conductivity and volumetric heat capacity of the cylinder material. The sensitivity coefficients and the determinant of the information matrix are examined for three different cylinders. The parameters with large and linearly independent sensitivity coefficients are estimated by using actual experimental data. The Levenberg-Marquardt Method, (Beck and Arnold, 1977; Ozisik and Orlande, 2000) of minimization of the least-squares norm is used as the estimation procedure.

2. Physical Problem and Mathematical Formulation

The physical problem under picture in this work involves the heating of a cylindrical body, immersed in a temperature controlled water bath. The body is assumed to be initially at the uniform temperature T_0. For $t > 0$, the body is heated by convection with the surrounding water, which is maintained at the constant temperature T_∞, with a uniform and constant heat transfer coefficient h_∞. The cylinder diameter is $2b$ and its thickness is $2L$, as illustrated in Fig 1. The cylinder thermophysical properties are assumed to be constant during the time elapsed for the cylinder to reach equilibrium with the surrounding water.

By taking into account axial and longitudinal symmetries, the mathematical formulation of the heat conduction problem in the cylindrical body is given by:

$$C\frac{\partial T(r,z,t)}{\partial t} = k\frac{\partial^2 T(r,z,t)}{\partial r^2} + k\frac{1}{r}\frac{\partial T(r,z,t)}{\partial r} + k\frac{\partial^2 T(r,z,t)}{\partial z^2} \tag{1.a}$$

With the following boundary conditions:

$$\frac{\partial T(0,z,t)}{\partial r} = 0 \tag{1.b}$$

$$k\frac{\partial T(b,z,t)}{\partial r} + h_\infty T(b,z,t) = T_\infty h_\infty \tag{1.c}$$

$$\frac{\partial T(r,0,t)}{\partial z} = 0 \tag{1.d}$$

$$k\frac{\partial T(r,L,t)}{\partial z} + h_\infty T(r,L,t) = T_\infty h_\infty \tag{1.e}$$

and with the initial condition given by:

$$T(r,z,0) = T_o \tag{1.f}$$

where k and C ($= \rho\, c_p$) are the thermal conductivity and volumetric heat capacity of the cylindrical body, respectively.

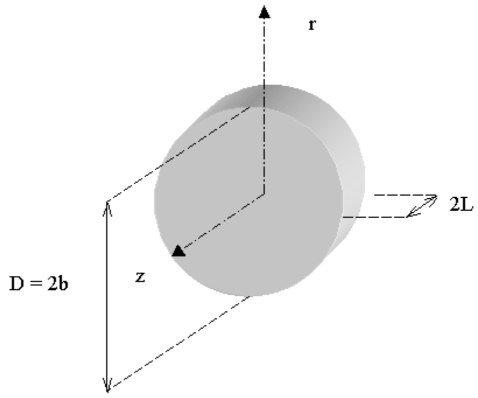


Figure 1. Body geometry

3. Direct Problem and Inverse Problem

In the *direct problem* associated with the mathematical formulation of the physical problem just described, the transient temperature field in the body is determined by assuming the physical properties, initial and boundary conditions and the geometrical characteristics of the body as known.

The *inverse problem* of interest for this work deals with the identification of the volumetric heat capacity (C), thermal conductivity (k) and heat transfer coefficient (h_∞), by using transient temperature measurements taken within the body. For the solution of the inverse problem, the initial temperature of the body (T_0), as well as the water temperature (T_∞) and the body geometry, are assumed to be known with high degree of accuracy. On the other hand, the temperature measurements may contain random errors.

The inverse problem under picture is a *parameter estimation problem*. For the solution of such inverse problem, we consider here the use of minimization techniques. An objective function is then defined, involving the difference between measured and estimated temperatures. In order to appropriately choose the objective function, some hypotheses regarding the measurement errors are required. Let us assume valid the following statistical hypotheses (Beck and Arnold, 1977): the errors in the measured variables are additive, uncorrelated, normally distributed, with zero mean and known constant standard-deviation; only the measured variables appearing in the objective function contain errors; and there is no prior information regarding the values and uncertainties of the unknown parameters. In this case, the ordinary least squares norm becomes a minimum variance estimator, Beck and Arnold (1977). The minimization of such objective function is described next.

3. Method of Solution for the Inverse Problem

The inverse problem of interest in this work deals with the estimation of the vector of unknown parameters through the minimization of the ordinary least squares norm, which is given by:

$$S_{OLS}(\mathbf{P}) = [\mathbf{Y} - \mathbf{T}(\mathbf{P})]^T [\mathbf{Y} - \mathbf{T}(\mathbf{P})] \tag{2}$$

where $\mathbf{P} = [\ k\ ,\ C\ ,\ h_\infty\ ]$ and

$$[\mathbf{Y} - \mathbf{T}(\mathbf{P})]^T = \left(\vec{Y}_1 - \vec{T}_1\ ,\ \vec{Y}_2 - \vec{T}_2\ , \ldots , \vec{Y}_I - \vec{T}_I\right) \tag{3.a}$$

The row vector $[\vec{Y}_i - \vec{T}_i]$ contains the difference between measured and estimated variables for each of the M sensors at time t_i, $i = 1, \ldots, I$, that is,

$$(\vec{Y}_i - \vec{T}_i) = \left(Y_{i1} - T_{i1}\ ,\ Y_{i2} - T_{i2}\ , \ldots , Y_{iM} - T_{iM}\right) \qquad \text{for } i=1,\ldots,I \tag{3.b}$$

The iterative procedure of the *Levenberg-Marquardt Method* for the minimization of the *ordinary least squares norm* expressed by Eq. (2) is used in this work. Such procedure is given by (Beck and Arnold, 1977; Ozisik and Orlande, 2000):

$$\mathbf{P}^{k+1} = \mathbf{P}^k + (\mathbf{J}^T\mathbf{J} + \lambda^k \mathbf{\Omega}^k)^{-1}\mathbf{J}^T[\mathbf{Y} - \mathbf{T}(\mathbf{P}^k)] \tag{4}$$

where k denotes the number of iterations, **J** is the sensitivity matrix, $\mathbf{\Omega}$ is a diagonal matrix and λ is a scalar named damping parameter (Beck and Arnold, 1977; Ozisik and Orlande, 2000). The purpose of the matrix term $\lambda^k\mathbf{\Omega}^k$ in Eq. (4) is to damp oscillations and instabilities due to the ill-conditioned character of the problem, by making its components large as compared to those of $\mathbf{J}^T\mathbf{J}$, if necessary. The damping parameter is made large in the beginning of the iterations. With such an approach, the matrix $\mathbf{J}^T\mathbf{J}$ is not required to be non-singular in the beginning of iterations and the Levenberg-Marquardt Method tends to the *Steepest Descent Method*, that is, a very small step is taken in the negative gradient direction. The parameter λ^k is then gradually reduced as the iteration procedure advances to the solution of the parameter estimation problem and then the Levenberg-Marquardt Method tends to the *Gauss Method*, (Beck et al, 1977). However, if the errors inherent to the measured data are amplified, generating instabilities on the solution as a result of the ill-conditioned character of the problem, the damping parameter is automatically increased. Such an automatic control of the damping parameter makes the Levenberg-Marquardt method a quite robust and stable estimation procedure, so that it does not require the use of the *Discrepancy Principle* in the stopping criterion to become stable, like the conjugate gradient method (Ozisik and Orlande, 2000).

The *Sensitivity matrix*, **J**, for a general case involving the estimation of N parameters, is defined as:

$$\mathbf{J(P)} \equiv \left[\frac{\partial \mathbf{T}^T(\mathbf{P})}{\partial \mathbf{P}}\right]^T = \begin{bmatrix} \frac{\partial \vec{T}_1^T}{\partial P_1} & \frac{\partial \vec{T}_1^T}{\partial P_2} & \frac{\partial \vec{T}_1^T}{\partial P_3} & \cdots & \frac{\partial \vec{T}_1^T}{\partial P_N} \\ \frac{\partial \vec{T}_2^T}{\partial P_1} & \frac{\partial \vec{T}_2^T}{\partial P_2} & \frac{\partial \vec{T}_2^T}{\partial P_3} & \cdots & \frac{\partial \vec{T}_2^T}{\partial P_N} \\ \vdots & \vdots & \vdots & & \vdots \\ \frac{\partial \vec{T}_I^T}{\partial P_1} & \frac{\partial \vec{T}_I^T}{\partial P_2} & \frac{\partial \vec{T}_I^T}{\partial P_3} & \cdots & \frac{\partial \vec{T}_I^T}{\partial P_N} \end{bmatrix} \tag{5.a}$$

where

$$\frac{\partial \vec{T}_i^T}{\partial P_j} = \begin{bmatrix} \frac{\partial T_{i1}}{\partial P_j} \\ \frac{\partial T_{i2}}{\partial P_j} \\ \vdots \\ \frac{\partial T_{iM}}{\partial P_j} \end{bmatrix} \quad \text{for } i = 1, \ldots, I \quad \text{and} \quad j = 1, \ldots, N \tag{5.b}$$

and I = number of transient measurements per sensor
M = number of sensors
N = number of unknown parameters

4. Statistical Analysis

By performing a *statistical analysis* it is possible to assess the accuracy of $\hat{P}_j$, which are the values estimated for the unknown parameters P_j, j=1,...,N. By assuming valid the statistical hypotheses about the measurement errors described above, the *covariance matrix*, of the estimated parameters $\hat{P}_j$, corresponding to the *ordinary least squares norm*, is given by (Beck and Arnold, 1977):

$$\mathbf{V} = \text{cov}(\hat{\mathbf{P}}) = (\mathbf{J}^T\mathbf{J})^{-1}\sigma^2 \tag{6}$$

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

$$\sigma_{\hat{P}_j} \equiv \sqrt{\text{cov}(\hat{P}_j, \hat{P}_j)} \qquad \text{for } j=1,\ldots,N \tag{7}$$

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

$$\hat{P}_j - 2.576\ \sigma_{\hat{P}_j} \le P_j \le \hat{P}_j + 2.576\ \sigma_{\hat{P}_j} \qquad \text{for } j=1,...,N \tag{8}$$

The joint confidence region for the estimated parameters is given by Beck and Arnold (1977):

$$(\hat{\mathbf{P}} - \mathbf{P})^T \mathbf{V}^{-1} (\hat{\mathbf{P}} - \mathbf{P}) \le \chi_N^2 \tag{9}$$

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

5. 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 Eq. (9) can be obtained by maximizing the determinant of $\mathbf{V}^{-1}$, in the so-called *D-optimum design* (Beck and Arnold, 1977). Since the covariance matrix is given by Eq. (8), we can then design optimum experiments by maximizing the determinant of the so-called *Fisher's Information Matrix*, $\mathbf{J}^T\mathbf{J}$ (Beck and Arnold, 1977). Therefore, optimal experimental variables, such as the duration of the experiment and the number of measurements, are chosen based on the criterion

$$\max \left| \mathbf{J}^T \mathbf{J} \right| \tag{10}$$

6. Experiments

The experiments involving the heating of a cylindrical body in a temperature-controlled water bath were conducted in the *Laboratory of Heat Transmission and Technology* (LTTC) of PEM/COPPE. In order to examine the effects of the material type and body dimensions on the estimated parameters, the experiments were run on three different specimens. The specimens' materials and dimensions are summarized in table 1. Each specimen was instrumented with two type-K thermocouples, which were located near the body lateral surface and the body center, respectively. The thermocouple locations are also presented in Tab. (1), by taking as reference the cylinder center, as illustrated in Fig. (1). The temperature readings were automatically recorded by using a data logger, with a frequency of 1 measurement per sensor per second. The three specimens are illustrated in Fig (2).

Table 1. Specimens' characteristics

Specimen	Material	Thickness (mm)	Diameter (mm)	Location of thermocouple 1* (r,z)	Location of thermocouple 2* (r,z)
1	Teflon	20.6	52.1	(0,0)	(0,8.4)
2	Teflon	9.4	51.6	(5.3,0)	(3.6,2.6)
3	Aluminum	72.7	28.6	(0,0)	(13.5,0)

* Taken as reference the cylinder center

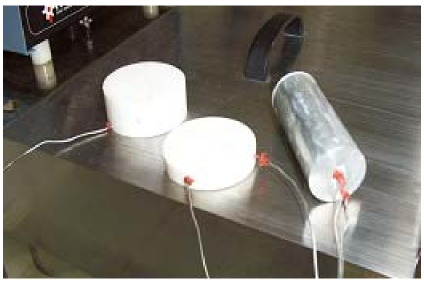


Figure 2. Specimen

In the experiments, the specimen, initially in equilibrium at room temperature, was fully immersed into the water. The time instant when the specimen was immersed was carefully recorded, in order to provide the time reference for the problem. The water temperature control in the bath was set to 50 ^{o}C, but during the experiments the water temperature was recorded in order to provide the T_∞ value for the boundary conditions in Eqs. (1.c,e). The experiment was run until the specimen was practically in thermal equilibrium with the water.

7. Results and Discussion

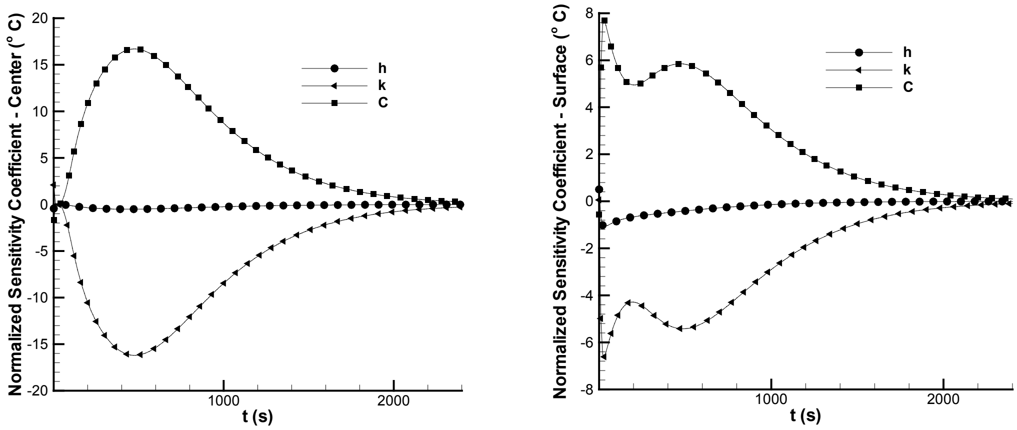
Before attempting to estimate the unknown parameters, let's first examine the sensitivity coefficients at each of the sensor locations in the three specimens, as well as the transient variation of the determinant of the information matrix. We note that, for nonlinear estimation problems such as the one under picture in this work, these analyses are not global, because these quantities are functions of the unknown parameters. Therefore, *a priori* estimated values for the parameters are required for the analyses of the sensitivity coefficients and of the determinant of the information matrix. Table 2 presents the values that were used for the parameters in these analyses for each of the specimens. The values for thermal conductivity and volumetric heat capacity were taken from literature values (Ozisik, 1989). Similarly, the values used for the heat transfer coefficient were calculated with correlations for forced convection around the cylinder (Ozisik, 1989).

Table 2. Values used for the analyses of the sensitivity coefficients and of the determinant of the information matrix

Specimen	k $(W/m\ K)$	C (J/m^3K)	h_∞ (W/m^2K)
1	0.23	2.3×10^6	1300
2	0.28	2.3×10^6	1500
3	204	2.4×10^6	1610

Figures 3.a,b present the normalized sensitivity coefficients with respect to each of the unknown parameters for specimen 1, at the locations of thermocouples 1 and 2, respectively. The normalized sensitivity coefficients were obtained by multiplying the original sensitivity coefficients by the parameters that they are referred to. These figures show that, for both thermocouple locations, the sensitivity coefficients with respect to the thermal conductivity and to the volumetric heat capacity are linearly dependent. Therefore, the simultaneous estimation of such two parameters is not possible in this case. Also, we notice in figures Figs. (3.a,b) that the sensitivity coefficient with respect to the heat transfer coefficient is quite small. As a result, the estimation of h_∞ is difficult and large confidence intervals are expected because of ill-conditioning of the matrix $\mathbf{J}^T\mathbf{J}$. Indeed, an analysis of equations (1.a-f) reveals that the three parameters actually appear in the mathematical formulation as the ratios k/C and h_∞/k. In fact, we could expect *a priori* that the simultaneous estimation of the three parameters would not be possible for the present case, but only of the ratios k/C and h_∞/k.

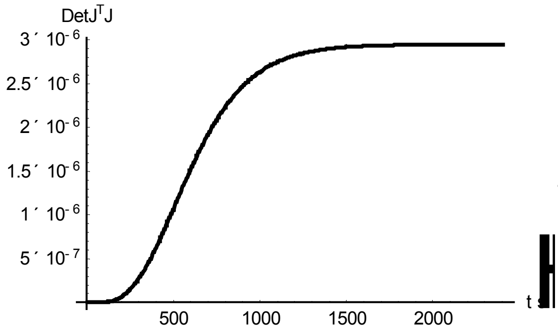
The qualitative behavior of the sensitivity coefficients for specimens 2 and 3 are very similar to those shown in Figs. (3.a,b). Therefore, for the sake of brevity, they are not presented here. We note, however, that the sensitivity coefficients obtained at the two thermocouple locations are practically identical for specimen 3. This is due to the very low Biot number because of the high thermal conductivity of aluminum, which result in a practically uniform temperature within the specimen. Furthermore, for specimen 2 the sensitivity coefficient with respect to the heat transfer coefficient is linearly-dependent with the two other sensitivity coefficients. Hence, for specimen 2 only one of the parameters can be estimated.



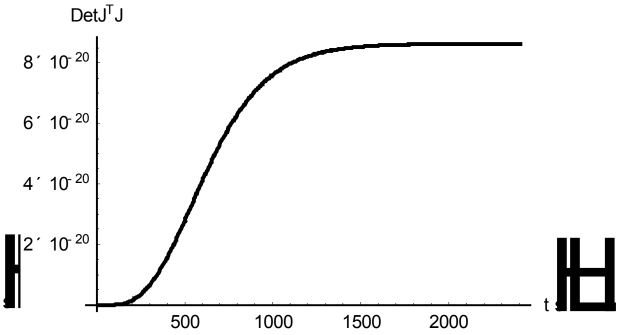
(a) (b)

Figures 3.a,b. Sensitivity coefficients for thermocouples 1 and 2, respectively – Specimen 1

The determinant of the information matrix, obtained for the estimation h_∞ and k and for the estimation of k and C, are shown in Figs. (4.a,b), respectively, for specimen 1. We note that such determinants increase until the specimen reaches thermal equilibrium with water, when the sensitivity coefficients tend to zero (see Figs (3.a,b)). Therefore, measurements taken after thermal equilibrium between the specimen and water has been reached are not useful for the parameter estimation. A comparison of figures 4.a and 4.b reveal that the determinant for the estimation of h_∞ and k is much larger than that for the estimation of k and C, for specimen 1. This is a result of the linear dependence between the sensitivity coefficients for k and C. The behavior for the determinant of the information matrix shown in figures 4.a,b is representative of those obtained for specimens 2 and 3. We note, however, that thermal equilibrium is reached much faster for specimen 3 because of the high thermal conductivity of aluminum.



(a)



(b)

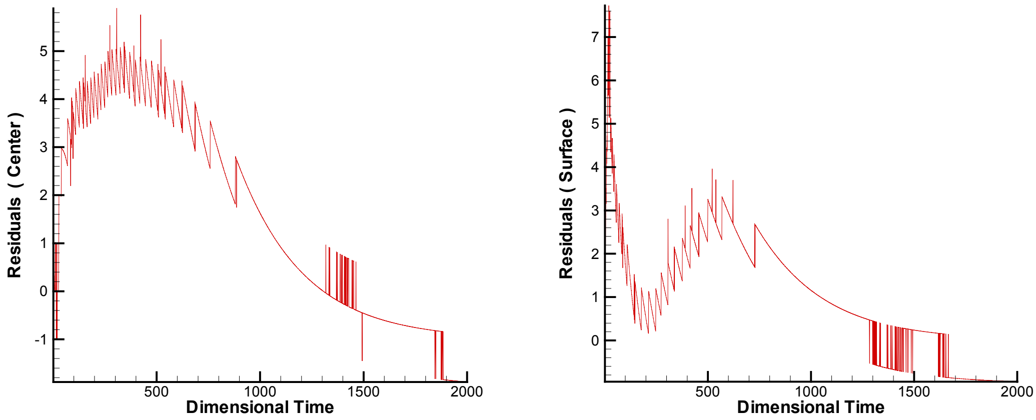
Figures 4.a,b. Determinant of the information matrix obtained for the estimation of h_∞ and k and for the estimation of k and C, respectively – Specimen 1

We present in Table (3) the values estimated simultaneously for h_∞ and k, for specimens 1 and 3, as well as the value estimated for k for specimen 2. The results presented in Tab. 3 were obtained by using the values of C (and h_∞, required only for specimen 2) presented in Table (2) in the inverse analysis. The 99% confidence intervals obtained for the parameters are also presented in this table. We note in Tab. (3) that the values estimated for the thermal conductivity of Teflon for specimens 1 and 2 are remarkably similar. The value estimated for the thermal conductivity of aluminum with specimen 3 is also in good agreement with the values found in the literature (Ozisik, 1989). Table (3) shows that, generally, the heat transfer coefficient is larger for specimen 3. This is probably caused by the geometry of this specimen, which is slender than those of specimens 1 and 2.

Table 3. Estimated parameters

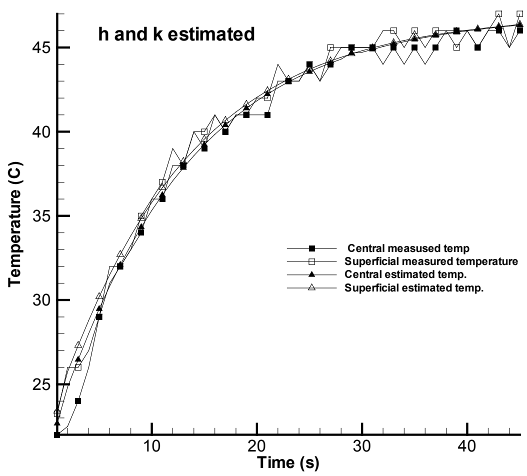
Specimen	k (W/mK)	h_∞ (W/m^2K)
1	0.27 ± 0.05	246 ± 157
2	0.299 ± 0.001	-
3	147 ± 3	1215 ± 3

The residuals obtained from the estimation of h_∞ and k for the two thermocouples with specimen 1 are presented in Fig. (5.a,b). An analysis of these figures reveals that the residuals are large and highly correlated. This gives an indication that the mathematical model used for the physical problem is not appropriate (Beck and Arnold, 1977). Also, uncertainties on the values used for the volumetric heat capacity, based on literature data, may have caused such a behavior of the residuals. Similar residuals were obtained with specimen 2. On the other hand, the agreement between measured and estimated temperatures is much better for specimen 3, as illustrated in Fig. (6).



(a) **(b)**

Figures 5.a,b. Residuals (ºC) versus time (seconds) for thermocouples 1 and 2, respectively – Specimen 1



Figures 6. Comparison between measured and estimated temperatures – Specimen 3

8. Conclusions

This paper presented the solution of the inverse parameter estimation problem involving the heating of cylindrical bodies in hot water. Experiments were run with three different cylinders, in order to examine the effects of size and material properties on the estimation results. From the parameters appearing in the mathematical formulation of the physical problem, except for specimen 2, the thermal conductivity and the heat transfer coefficient exhibited linearly independent sensitivity coefficients, and were selected as unknown. The values estimated for thermal conductivity are in good agreement with those available in the literature. Despite such a result, the temperature residuals were large and highly correlated, specially for specimens 1 and 2. This result motivated the solution of the inverse problem as a function estimation approach, as described in Part II of this paper.

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