SEQUENTIAL ESTIMATION OF THERMAL CONDUCTIVITY AND VOLUMETRIC HEAT CAPACITY

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Abstract. *This paper deals with the sequential estimation procedure for the identification of thermal conductivity and of volumetric heat capacity of solids. The experimental setup conceived consists of a heater symmetrically assembled between two pieces of the specimen with unknown properties. The sequential estimation procedure is described in detail, as applied to the present nonlinear parameter estimation problem. Transient simulated temperature measurements taken in the specimen are used in order to verify the accuracy of this estimation approach.*

Keywords: *Thermal Conductivity, Volumetric Heat Capacity, Sequential Parameter Estimation, Maximum a Posteriori Estimator*

1. INTRODUCTION

The accurate knowledge of thermophysical properties is of importance for the correct prediction of the thermal behavior of bodies. Several experimental techniques have been developed in the past for the estimation of thermal conductivity and thermal diffusivity, by using steady-state, as well as transient experiments. Such techniques include, among others, the guarded hot-plate method (ASTM, C177), the Flash method (Taylor and Maglic, 1984) and the hot-wire method (Blackwell, 1954). Transient techniques have the advantage of involving faster experiments than steady-state techniques.

More recently, the use of inverse analysis techniques of parameter estimation have been used for the identification of thermophysical properties, by utilizing minimization procedures involving transient measurements (Taktak et al, 1993, Dowding et al, 1995, 1996, Orlande et al, 1994, 1995, Guimarães et al, 1997, Mejias et al, 1999, Oliveira et al, 1999). More specifically, in a previous paper we discussed the design of optimum experiments for the simultaneous estimation of thermal conductivity and volumetric heat capacity of solids (Oliveira et al, 1999). Three possible arrangements for the experimental setup, involving a heater placed between two identical pieces of the specimen with unknown properties, were examined in such work. The arrangement resulting on smaller confidence regions for the parameters was that involving a constant temperature boundary condition for the non-heated surface. The Levenberg-Marquardt method (Beck and Arnold, 1977, Ozisik and Orlande, 2000) was used for the minimization of the least-squares norm. The accuracy of such a parameter estimation approach was verified by using transient simulated measurements containing random errors.

The main objectives of this work are to implement and test the *Sequential Estimation Procedure* advanced by Beck (1977, 1999) for the identification of thermal conductivity and volumetric heat capacity, in an experimental setup similar to that designed by Oliveira et al (1999). Such a sequential procedure uses previously estimated values for the unknown parameters in order to obtain improved estimates. An analysis of the values estimated sequentially permit the identification of improper mathematical models used for the physical problem under picture. Also, with such an approach it is possible to identify if a sufficient number of transient measurements and if a sufficiently long experimental time have been used in the experiment in order to obtain accurate estimates for the unknown parameters.

2. PHYSICAL PROBLEM AND MATHEMATICAL FORMULATION

The physical problem considered here, involving the experimental apparatus to be used for the simultaneous estimation of thermal conductivity and volumetric heat capacity, consists of a heater symmetrically placed between two identical pieces of length L, of the solid with unknown properties. The heater is turned on for a period $0 < t \le t_h$. Transient temperature measurements taken in the solid in the period $0 < t \le t_f$, where $t_h \le t_f$, are used for the estimation of the properties.

In a previous work, we examined the effects of the boundary condition at the non-heated surface at $x = L$ on the accuracy of the estimated parameters (Oliveira et al, 1999). The use of a constant temperature boundary condition resulted on the largest values for the determinant of the Fisher information matrix and, consequently, on the smallest confidence regions for the estimated parameters. Therefore, in the present work we assume that the non-heated boundary at $x = L$ is kept at a constant temperature.

By taking into account the symmetry of the experimental apparatus, the mathematical formulation of the physical problem examined here is given in dimensionless form as

$$c^* \frac{\partial \theta}{\partial \tau} = k^* \frac{\partial^2 \theta}{\partial X^2}, \qquad \text{in } 0 < X < 1, \text{ for } \tau > 0 \tag{1.a}$$

$$k^* \frac{\partial \theta}{\partial X} = -u(\tau_h - \tau), \qquad \text{at } X = 0, \text{ for } \tau > 0 \tag{1.b}$$

$$\theta = 0, \qquad \text{at } X = 1, \text{ for } \tau > 0 \tag{1.c}$$

$$\theta = 0, \qquad \text{in } 0 < X < 1, \text{ for } \tau = 0 \tag{1.d}$$

where:

$$u(\tau_h - \tau) = \begin{cases} 1, & 0 < \tau \le \tau_h \\ 0, & \tau > \tau_h \end{cases} \tag{2}$$

and the following dimensionless variables were defined:

$$X = \frac{x}{L}, \; \tau = \frac{k_R}{\rho c_R L^2} t, \; k^* = \frac{k}{k_R}, \; c^* = \frac{c}{c_R}, \; \theta = \frac{k_R}{q_0 L}(T - T_0) \tag{3.a-e}$$

In equations (3), k_R and c_R are reference values for thermal conductivity and volumetric heat capacity, respectively, ρ is the density of the solid, q_0 is the magnitude of the applied heat flux during the period $0 < t \le t_h$ and T_0 is the constant temperature at the boundary $x = L$, which is also assumed to be the initial temperature in the region.

Problem (1), with known thermophysical properties, boundary and initial conditions, constitutes a *Direct Heat Conduction Problem*. The analytical solution for this direct problem can be easily obtained *via* the Classical Integral Transform Technique (Ozisik, 1993) as:

$$\theta(X,\tau) = \sum_{m=1}^{\infty} 2\cos(\lambda_m X) \left\{ \frac{1}{k^* \lambda_m^2} \left(1 - e^{-\frac{k^*}{c^*}\lambda_m^2 \tau} \right) \right\} \qquad \text{For} \quad 0 < \tau \le \tau_h , \tag{4.a}$$

and

$$\theta(X,\tau) = \sum_{m=1}^{\infty} 2\cos(\lambda_m X) \left\{ \frac{1}{k^* \lambda_m^2} \left(e^{\frac{k^*}{c^*}\lambda_m^2 (\tau_h - \tau)} - e^{-\frac{k^*}{c^*}\lambda_m^2 \tau} \right) \right\} \qquad \text{For} \quad \tau > \tau_h , \tag{4.b}$$

where:

$$\lambda_m = (2m-1)\pi/2 \tag{5}$$

3. INVERSE PROBLEM

For the *Inverse Problem* considered here, the thermal conductivity *k** and the volumetric heat capacity *c** are regarded as unknown quantities. For the estimation of such properties, we consider available for the inverse analysis the transient readings Y_i taken at times t_i, $i = 1,...,I$, of one temperature sensor located in the solid with unknown properties.

Such type of inverse parameter estimation problem is usually solved through the minimization of the least-squares norm, in a whole-domain approach, where all the transient measurements are used simultaneously in the minimization procedure (Beck and Arnold, 1977, Ozisik and Orlande, 2000). In this paper, we use an alternative approach where the parameters are estimated by using the transient measurements Y_i, for t_i, $i = 1,...,I$, sequentially in time (Beck and Arnold, 1977, Beck, 1999), as described next.

4. SEQUENTIAL PARAMETER ESTIMATION

The starting point for the *Sequential Parameter Estimation Approach* advanced by Beck (1977, 1999) is the minimization of the *Maximum a Posteriori* objective function. Such objective function, for the estimation of the vector of unknown parameters $\mathbf{P}=[k^*,c^*]$, is defined as (Beck and Arnold, 1977):

$$S(\mathbf{P}) = [\mathbf{Y} - \mathbf{T}(\mathbf{P})]^T \mathbf{W} [\mathbf{Y} - \mathbf{T}(\mathbf{P})] + (\boldsymbol{\mu} - \mathbf{P})^T \mathbf{V}^{-1} (\boldsymbol{\mu} - \mathbf{P}) \tag{6.a}$$

where **W** is a weighting matrix and

$$[\mathbf{Y} - \mathbf{T}(\mathbf{P})]^T = [Y_1 - T_1(\mathbf{P}), Y_2 - T_2(\mathbf{P}), ..., Y_I - T_I(\mathbf{P})] \tag{6.b}$$

is the vector containing the differences between measured (Y_i) and estimated (T_i) temperatures.

The use of the *maximum a posteriori* objective function involves the following statistical assumptions (Beck and Arnold, 1977):

- The errors are additive and normally distributed with a zero mean;
- The statistical parameters describing the errors are known;
- There are no errors in the independent variables, such as time;
- **P** is a random vector with known mean μ and known covariance matrix **V**. **P** is distributed normally and **P** and **V** are uncorrelated.

We note that the above hypotheses do not involve any assumptions regarding the errors being uncorrelated or not, and the covariance matrix of the errors being constant or not.

The minimization of S(**P**) requires that its gradient be null. Thus,

$$\nabla S(\mathbf{P}) = -2\mathbf{J}^{T}\mathbf{W}[\mathbf{Y}-\mathbf{T}] - 2\mathbf{V}^{-1}(\boldsymbol{\mu}-\mathbf{P}) = 0 \tag{7}$$

By linearizing the vector of estimated temperatures with a Taylor series expansion around the estimated parameters at iteration k, that is,

$$\mathbf{T}(\mathbf{P}) = \mathbf{T}(\mathbf{P}^{k}) + \mathbf{J}^{k}(\mathbf{P}-\mathbf{P}^{k}) \tag{8}$$

we can write an iterative procedure for the estimation of the parameters **P** in the form (Beck and Arnold, 1977):

$$\mathbf{P}^{k+1} = \mathbf{P}^{k} + [\mathbf{J}^{T}\mathbf{W}\mathbf{J} + \mathbf{V}^{-1}]^{-1}\{\mathbf{J}^{T}\mathbf{W}[\mathbf{Y}-\mathbf{T}(\mathbf{P}^{k})] + \mathbf{V}^{-1}(\boldsymbol{\mu}-\mathbf{P}^{k})\} \tag{9}$$

where **J** is the *sensitivity matrix* defined as

$$\mathbf{J}(\mathbf{P}) = \left[\frac{\partial \mathbf{T}^{T}(\mathbf{P})}{\partial \mathbf{P}}\right]^{T} = \begin{bmatrix} \frac{\partial T_1}{\partial k^*} & \frac{\partial T_1}{\partial c^*} \\ \frac{\partial T_2}{\partial k^*} & \frac{\partial T_2}{\partial c^*} \\ \vdots & \vdots \\ \frac{\partial T_I}{\partial k^*} & \frac{\partial T_I}{\partial c^*} \end{bmatrix} \tag{10.a}$$

For convenience in the analysis, we write the sensitivity matrix as

$$\mathbf{J}(\mathbf{P}) = \begin{bmatrix} \mathbf{J}_1 \\ \mathbf{J}_2 \\ \vdots \\ \mathbf{J}_I \end{bmatrix} \tag{10.b}$$

where

$$\mathbf{J}_i = \left[\frac{\partial T_i}{\partial k^*}, \frac{\partial T_i}{\partial c^*}\right] \tag{10.c}$$

The elements of the sensitivity matrix are denoted as the *sensitivity coefficients*. They provide a measure of the sensitivity of the estimated (or measured) temperatures with respect to changes in the unknown parameters. Clearly, the solution of inverse problems involving sensitivity coefficients with small magnitudes is extremely difficult, because the choice of very different values for the unknown parameters would result in basically the same value for the measured variables. Also, the columns of the sensitivity matrix are required to be linearly independent in order to have the matrix $\mathbf{J}^T\mathbf{J}$ invertible, that is, the determinant of $\mathbf{J}^T\mathbf{J}$ cannot be zero or even very small. We note that analytical expressions can be easily obtained for the sensitivity coefficients, by differentiating equations (4.a,b) with respect to k* and c*.

If we make the additional assumption that the measurement errors are uncorrelated, the weighting matrix is given by

$$\mathbf{W} = \begin{bmatrix} W_1 & 0 & \cdots & 0 \\ 0 & W_2 & & \vdots \\ \vdots & & \ddots & 0 \\ 0 & \cdots & 0 & W_I \end{bmatrix} \tag{11.a}$$

where

$$\mathrm{W_i} = 1/\sigma_i^2 \qquad \text{for i=1,…,I} \tag{11.b}$$

and σ_i is the standard deviation of the measurement Y_i.

For the sequential nonlinear estimation, such as the one under picture in this paper, Beck and Arnold (1977) recommend that the parameters be initially estimated by using all measurements simultaneously. Afterwards, the problem is solved once more, this time sequentially, by using the parameters estimated simultaneously and its covariance matrix in the place of μ and $\mathbf{V}$, respectively.

In order to apply the sequential estimation approach, the linearization is performed around $\mathbf{P}^k$, which is taken as

$$\begin{aligned} \mathbf{P}^0 &= \boldsymbol{\mu} \qquad \text{for k} = 0 \\ \mathbf{P}^k &= \mathbf{P}_I^k \qquad \text{for k} = 1,2,... \end{aligned} \tag{12}$$

where $\mathbf{P}_I^k$ is the vector with the values estimated sequentially for the parameters at iteration k, obtained by using all I measurements.

The main steps for the computational algorithm of the sequential estimation approach can be organized as follows:

Step 1. Initialize the procedure with $k = 0$ and

$$\mathbf{P}^0 = \boldsymbol{\mu} \tag{13.a}$$
$$\mathbf{C}^0 = \mathbf{V}^{-1} \tag{13.b}$$
$$\mathbf{D}^0 = \mathbf{V}^{-1}(\boldsymbol{\mu} - \mathbf{P}^k) \tag{13.c}$$

Step 2. Compute the estimate for the vector of unknown parameters sequentially, for $i = 1,..., I$ with

$$\mathbf{P}_i^{k+1} = \mathbf{P}^k + \mathbf{C}_i^{-1}\mathbf{D}_i \tag{14.a}$$

where

$$\mathbf{C}_i = \mathbf{C}_{i-1} + \mathbf{J}_i^T \mathbf{W}_i \mathbf{J}_i \tag{14.b}$$

$$\mathbf{D}_i = \mathbf{D}_{i-1} + \mathbf{J}_i^T \mathbf{W}_i [\mathbf{Y}_i - \mathbf{T}_i(\mathbf{P}^k)] \tag{14.c}$$

Step 3. Check convergence with the values estimated sequentially with all I measurements, that is,

$$\left\| \mathbf{P}_I^{k+1} - \mathbf{P}_I^k \right\| < \varepsilon \tag{15.a}$$

If the criterion given by equation (15.a) is not satisfied, increment k, make

$$\mathbf{P}^k = \mathbf{P}_I^k \tag{15.b}$$

and return to **Step 2**.

The above computational algorithm is not in a suitable form for computational implementation. A more convenient form can be obtained by writing the sequential estimation explicitly, that is, the estimate for the vector of parameters $\mathbf{P}_i^{k+1}$, obtained with measurements up to time t_i at iteration k+1, is obtained directly from the estimate obtained with measurements up to time t_{i-1} at the same iteration, $\mathbf{P}_{i-1}^{k+1}$, instead of $\mathbf{P}^k$ as in equation (14.a).

In order to derive such alternative form for the sequential estimation procedure we rewrite equation (14.a) for the $(k+1)^{th}$ iteration, with measurements up to time i+1, as:

$$\mathbf{P}_{i+1}^{k+1} = \mathbf{P}^k + [\mathbf{J}_{i+1}^T \mathbf{W}_{i+1} \mathbf{J}_{i+1} + \mathbf{C}_i]^{-1} \{\mathbf{J}_{i+1}^T \mathbf{W}_{i+1} [\mathbf{Y}_{i+1} - \mathbf{T}_{i+1}(\mathbf{P}^k)] + \mathbf{D}_i\} \tag{16.a}$$

or, alternatively,

$$[\mathbf{J}_{i+1}^T \mathbf{W}_{i+1} \mathbf{J}_{i+1} + \mathbf{C}_i][\mathbf{P}_{i+1}^{k+1} - \mathbf{P}^k] = \mathbf{J}_{i+1}^T \mathbf{W}_{i+1} [\mathbf{Y}_{i+1} - \mathbf{T}_{i+1}(\mathbf{P}^k)] + \mathbf{D}_i \tag{16.b}$$

By subtracting $[\mathbf{J}_{i+1}^T \mathbf{W}_{i+1} \mathbf{J}_{i+1} + \mathbf{C}_i]\mathbf{P}_i^{k+1}$ from both sides of equation (16.b) and after performing some algebraic manipulations we obtain:

$$\mathbf{P}_{i+1}^{k+1} = \mathbf{P}_i^k + \mathbf{V}_{i+1} \mathbf{J}_{i+1}^T \mathbf{W}_{i+1} \{[\mathbf{Y}_{i+1} - \mathbf{T}_{i+1}(\mathbf{P}^k)] - \mathbf{J}_{i+1} [\mathbf{P}_i^{k+1} - \mathbf{P}^k]\} \tag{17.a}$$

where

$$\mathbf{V}_{i+1} = [\mathbf{J}_{i+1}^T \mathbf{W}_{i+1} \mathbf{J}_{i+1} + \mathbf{C}_i]^{-1} \tag{17.b}$$

$\mathbf{V}_{i+1}$ is the covariance matrix for the linear *maximum a posteriori* estimator using i+1 measurements, which is used as an approximation for the nonlinear estimator (Beck and Arnold, 1977).

By using the following matrix identities (Beck and Arnold, 1977):

$$\begin{aligned} \mathbf{V}_{i+1} &= \mathbf{V}_i - \mathbf{V}_i \mathbf{J}_{i+1}^T (\mathbf{J}_{i+1} \mathbf{V}_i \mathbf{J}_{i+1}^T + \mathbf{W}_{i+1}^{-1})^{-1} \mathbf{J}_{i+1} \mathbf{V}_i \\ \mathbf{V}_{i+1} \mathbf{J}_{i+1}^T \mathbf{W}_{i+1} &= \mathbf{V}_i \mathbf{J}_{i+1}^T (\mathbf{J}_{i+1} \mathbf{V}_i \mathbf{J}_{i+1}^T + \mathbf{W}_{i+1}^{-1})^{-1} \end{aligned} \tag{18.a,b}$$

where equation (18.a) is referred to as the *Matrix Inversion Lemma* (Beck and Arnold, 1977, Beck, 1999), we can write the following computational algorithm for the sequential estimation approach:

Step 1. Initialize the procedure with $k = 0$ and

$$\mathbf{P}^0 = \boldsymbol{\mu} \tag{19}$$

Step 2. Compute the estimate for the vector of unknown parameters sequentially, for $i = 0,...,I-1$ with

$$\mathbf{A} = \mathbf{V}_i \, \mathbf{J}_{i+1}^T \tag{20.a}$$

$$\boldsymbol{\Delta} = \mathbf{J}_{i+1} \, \mathbf{A} + \mathbf{W}_{i+1}^{-1} \tag{20.b}$$

$$\mathbf{K} = \mathbf{A} \, \boldsymbol{\Delta}^{-1} \tag{20.c}$$

$$\mathbf{E}_{i+1} = \mathbf{Y}_{i+1} - \mathbf{T}_{i+1}(\mathbf{P}^k) \tag{20.d}$$

$$\mathbf{P}_{i+1}^{k+1} = \mathbf{P}_i^{k+1} + \mathbf{K}[\mathbf{E}_{i+1} - \mathbf{J}_{i+1}(\mathbf{P}_i^{k+1} - \mathbf{P}^k)] \tag{20.e}$$

$$\mathbf{V}_{i+1} = \mathbf{V}_i - \mathbf{K} \, \mathbf{J}_{i+1} \mathbf{V}_i \tag{20.f}$$

where

$$\mathbf{V}_0 = \mathbf{V} \tag{20.g}$$

$$\mathbf{P}_0^k = \boldsymbol{\mu} \tag{20.h}$$

Step 3. Check convergence with the values estimated sequentially with all I measurements, that is,

$$\left\| \mathbf{P}_I^{k+1} - \mathbf{P}_I^k \right\| < \varepsilon \tag{21.a}$$

If the criterion given by equation (21.a) is not satisfied, increment k, make

$$\mathbf{P}^k = \mathbf{P}_I^k \tag{21.b}$$

and return to step 2.

A quite important computational feature of the above algorithm is that, if one measurement is added at a time, such as for the case involving transient measurements of a single sensor, no matrix inversion is performed because $\boldsymbol{\Delta}$ and $\mathbf{W}_{i+1}$ are scalars. In fact, even if transient measurements of multiple sensors are used in the analysis, they can be arranged so that one single measurements is added to the sequential estimation at a time, so that no matrix inversions need to be performed.

The above computational algorithm was derived for a case where previous estimates were available for the vector of parameters and for their covariance matrix, obtained by using all measurements simultaneously, i.e., not sequentially. However, it can also be used for cases where no previous estimations are available, or if available, they have large uncertainty. For such cases, we take $\boldsymbol{\mu}$ as any vector, say, with null components. Also, we take $\mathbf{V}$ as a diagonal matrix with large values on the diagonal as compared to the square of the expected values for the parameters.

5. RESULTS AND DISCUSSIONS

We present below the results obtained with the sequential estimation approach described in this paper, for the estimation of k* and c*, obtained with simulated measurements. Such simulated measurements were obtained from the solution of the direct problem (1) for $k^* = c^* = 1$. The measurements obtained in such manner are considered as exact. Measurements containing random errors were generated by adding a noise term with normal distribution, zero mean and constant standard-deviation to these exact values.

For the cases examined here, the sensor was located at $X = 0$. Such location was the one resulting on the largest values of the determinant of the Fischer information matrix, and consequently, on the smaller confidence intervals for the estimated parameters (Oliveira et al, 1999). Similarly, we used here $\tau_h = 2.2$ and $\tau_f = 3.0$.

Table 1 illustrates the results obtained with the sequential estimation approach, after the parameters and their covariance matrix have been initially estimated with the Levenberg-Marquardt method, for different number of transient measurements used in the analysis. We note that for the cases presented in Table 1, no improvement on the accuracy of the estimated parameters was obtained by using the sequential approach, after the parameters were initially estimated with the Levenberg-Marquartd method. This is the case because the parameters were initially estimated with optimally-designed variables, resulting on minimum variance estimates. In fact, the parameters estimated sequentially converged immediately to the parameters estimated with the Levenberg-Marqaurdt method, as shown in Figure 1.

Table 1. Sequentially estimated parameters with *a priori* information

I		Levenberg-Marquardt		Sequential Estimation	
		Estimated Parameter	Standard Deviation	Estimated Parameter	Standard Deviation
50	k*	0.999	0.002	0.999	0.002
	c*	1.011	0.007	1.011	0.007
100	k*	1.001	0.001	1.001	0.001
	c*	1.006	0.005	1.006	0.005
150	k*	1.000	0.001	1.000	0.001
	c*	1.006	0.004	1.006	0.004

We now examine a case where no prior information regarding the values for the parameters and for their covariance matrix was assumed available. In this case, we took $k^* = c^* = 10^{-10}$ as the initial guesses for the parameters and $V_{11} = V_{22} = 100$. Figure 2 shows the results obtained for the sequentially estimated parameters with different number of transient measurements. Similarly to the case examined above, optimally designed values were used for τ_h and τ_f, and the single sensor was located at $X = 0$. These figures show that the parameters converged fast to their exact values during the experimental time used for the analysis, even with a small number of transient measurements such as 50, when no *a priori* information was available regarding their values and variances.

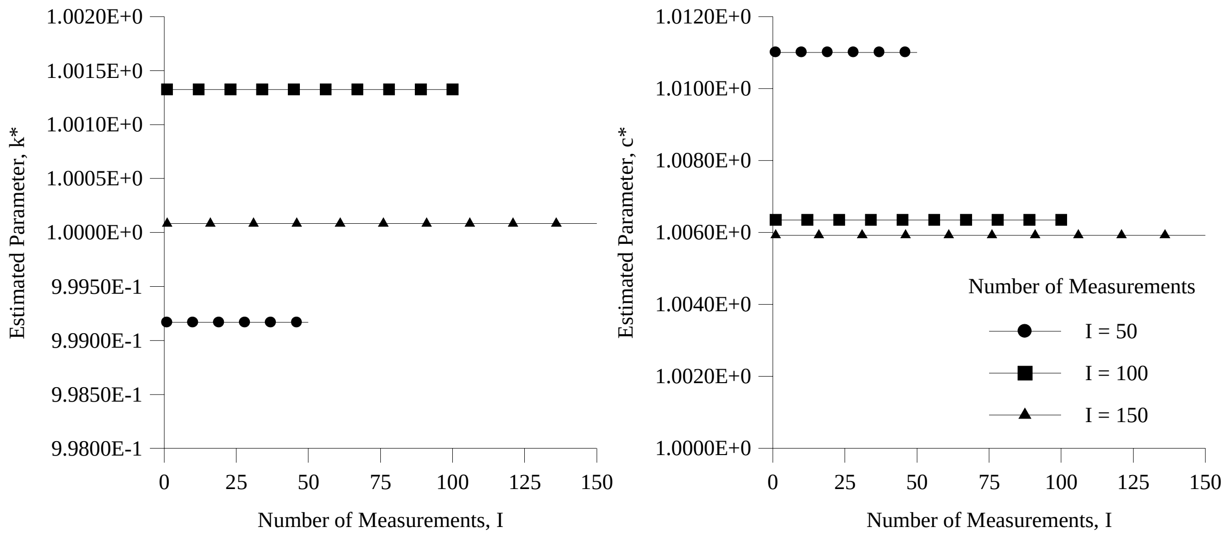

Figure 1. Sequentially estimated k* and c* with *a priori* information

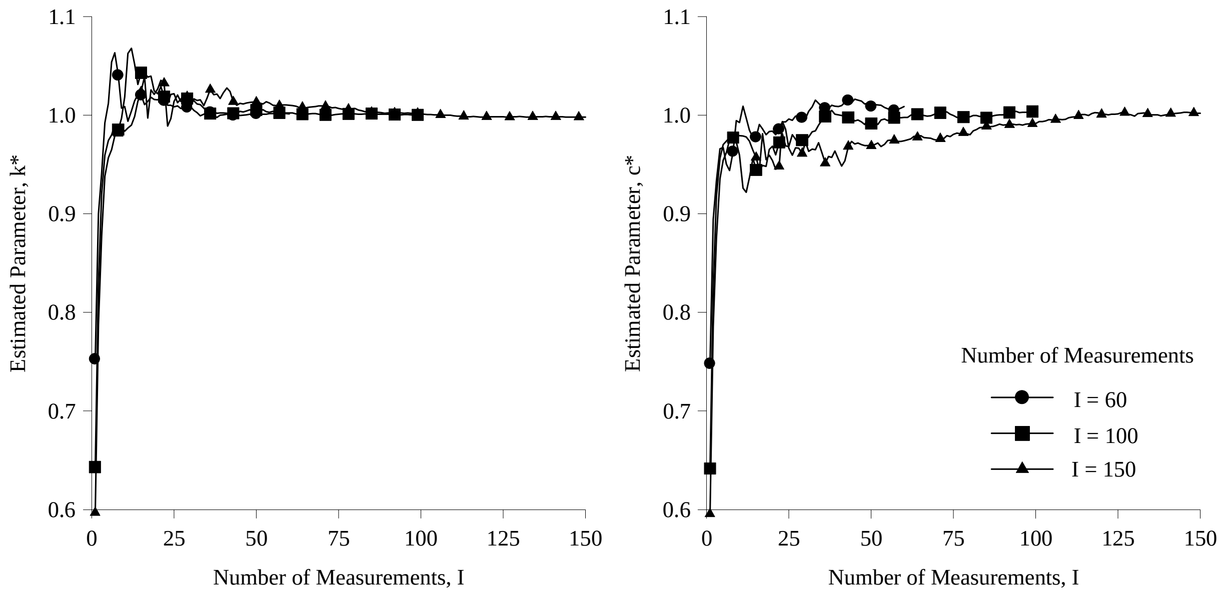

Figure 2. Sequentially estimated k* and c*with no *a priori* information

6. CONCLUSIONS

In this paper we described in detail and implemented Beck's sequential estimation procedure of parameter estimation. Test-cases involving the simultaneous estimation of thermal conductivity and volumetric heat capacity of solids were examined. No improvement on the accuracy of the estimated parameters was observed when *a priori* information was available from experiments optimally designed, but the sequential estimation procedure shows that the parameters converge to their exact values even with a small number of transient measurements. Parameters obtained sequentially also converged quite fast when no *a priori* information was assumed for the analysis, even when initial guesses very far from the exact values were used.

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