A COMPARISON OF DIFFERENT PARAMETER ESTIMATION TECHNIQUES FOR THE IDENTIFICATION OF THERMAL CONDUCTIVITY COMPONENTS OF ORTHOTROPIC SOLIDS

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ABSTRACT

In this paper we examine the inverse problem of identification of the three thermal conductivity components of an orthotropic cube. For the solution of such parameter estimation problem, we consider two different versions of the Levenberg-Marquardt method and four different versions of the conjugate gradient method. The techniques are compared in terms of rate of reduction of the objective function with respect to the number of iterations, CPU time and accuracy of the estimated parameters. Simulated measurements with and without measurement errors are used in the analysis, for three different sets of exact values for the parameters.

NOMENCLATURE

- *I* number of transient measurements per sensor
- J sensitivity coefficients
- **J** sensitivity matrix defined by equation (7)
- k_1,k_2,k_3 thermal conductivities in the x, y and z directions, respectively
- *M* number of sensors
- **P** vector of unknown parameters
- *S* least-squares norm defined by equation (5)
- T vector of estimated temperatures
- t_h , t_f heating time and final time
- Y vector of measured temperatures

GREEKS

 σ standard deviation of the measurement errors

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INTRODUCTION

In nature, several materials have direction-dependent thermal conductivities including, among others, woods and crystals. This is also the case for some man-made materials, for example, composites. Such kind of materials is denoted *anisotropic*, as an opposition to *isotropic* materials, in which the thermal conductivity does not vary with direction. A special case of anisotropic materials involve those where the offdiagonal elements of the conductivity tensor are null and the diagonal elements are the *principal conductivities* along three mutually orthogonal directions. They are referred to as *orthotropic* materials (Ozisik, 1993).

As a result of the importance of orthotropic materials in nowadays engineering, a lot of attention has been devoted in the recent past to the estimation of their thermal properties, by using inverse analysis techniques of parameter estimation (Sawaf and Ozisik, 1995, Sawaf et al, 1995, Taktak et al, 1993, Taktak, 1992, Dowding et al, 1995, 1996, Mejias et al, 1999).

In this paper we present a comparison of different methods of parameter estimation, as applied to the identification of the three thermal conductivity components of an orthotropic solid, by using simulated experimental data. Such a physical problem was chosen for comparison of the methods because it requires non-linear estimation procedures, since the sensitivity coefficients are functions of the unknown parameters. Experimental variables used in the analysis, such as the duration of the experiment, location of sensors and boundary conditions, were optimally chosen (Mejias et al, 1999). The methods examined in this work include: the *Levenberg-Marquardt Method* (Levenberg, 1944, Marquardt, 1963, Beck and Arnold, 1977, Moré, 1977, Mejias et al, 1999, Ozisik and Orlande, 1999) and the *Conjugate Gradient Method* versions of Fletcher-Reeves, Polak-Ribiere, Powell-Beale and Hestenes-Stieffel (Alifanov, 1994, Daniel, 1971, Ozisik and Orlande, 1999, Powell, 1977, Hestenes and Stiefel, 1952, Fletcher and Reeves, 1964, Colaço and Orlande, 1999). Such methods are compared in terms of the rate of reduction of the objective function, accuracy of estimated parameters and effects of the initial-guess on the convergence. Different sets of values are used for the thermal conductivity components in order to generate the simulated measurements, thus representing several practical engineering materials (Mejias et al, 1999), as described next.

DIRECT PROBLEM

The physical problem considered here involves the threedimensional linear heat conduction in an orthotropic solid, with thermal conductivity components k_1 , k_2 and k_3 in the x, y and z directions, respectively. The solid is considered to be a parallelepiped with sides a, b and c, initially at zero temperature. For times t > 0, uniform heat fluxes $q_1(t)$, $q_2(t)$ and $q_3(t)$ are supplied at the surfaces x = a, y = b and z = c, respectively, while the other three remaining boundaries at x = 0, y = 0 and z = 0 are supposed insulated. The mathematical formulation of such physical problem is given in dimensionless form by

$$k_1 \frac{\partial^2 T}{\partial x^2} + k_2 \frac{\partial^2 T}{\partial y^2} + k_3 \frac{\partial^2 T}{\partial z^2} = \frac{\partial T}{\partial t}$$

in $0 < x < a$, $0 < y < b$, $0 < z < c$; $t > 0$ (1.a)

$$\frac{\partial T}{\partial x} = 0$$
 at $x = 0$; $k_1 \frac{\partial T}{\partial x} = q_1(t)$ at $x = a$, for $t > 0$ (1.b,c)

$$\frac{\partial T}{\partial y} = 0$$
 at $y = 0$; $k_2 \frac{\partial T}{\partial y} = q_2(t)$ at $y = b$, for $t > 0$ (1.d,e)

$$\frac{\partial T}{\partial z} = 0$$
 at $z = 0$; $k_3 \frac{\partial T}{\partial z} = q_3(t)$ at $z = c$, for $t > 0$ (1.f,g)

$$T = 0$$
 for $t = 0$; in $0 \le x \le a$, $0 \le y \le b$, $0 \le z \le c$ (1.h)

In the *direct problem* associated with the physical problem described above, the three thermal conductivity components k_1 , k_2 and k_3 , as well as the solid geometry, initial and boundary conditions, are known. The objective of the direct problem is then to determine the transient temperature field T(x, y, z, t) in the body.

By following the same approach of Taktak et al (1993), we assume the boundary heat fluxes to be pulses of finite duration t_h , that is,

$$q_{j}(t) = \begin{cases} \overline{q}_{j} &, \text{ for } 0 < t \le t_{h} \\ 0 &, \text{ for } t > t_{h} \end{cases} \quad \text{for } j=1,2,3 \quad (2)$$

where \overline{q}_{j} is the dimensionless magnitude of the applied heat flux.

The solution of problem (1) with boundary heat fluxes given by equation (2), can be obtained analytically as a

superposition of three one-dimensional solutions by using the split-up procedure (Mikhailov and Ozisik, 1994) for $0 < t \le t_h$. We obtain for $0 < t \le t_h$

$$T(x, y, z, t) = \frac{\overline{q}_1 \ a}{k_1} \ \theta_1\left(\frac{x}{a}, \frac{k_1 \ t}{a^2}\right) + \frac{\overline{q}_2 \ b}{k_2} \ \theta_1\left(\frac{y}{b}, \frac{k_2 \ t}{b^2}\right) + \frac{\overline{q}_3 \ c}{k_3} \ \theta_1\left(\frac{z}{c}, \frac{k_3 \ t}{c^2}\right)$$
(3.a)

where

$$\theta_{1}(\xi,\tau) = -\frac{1}{6} + \frac{\xi^{2}}{2} + \tau +$$

+ $\sum_{i=1}^{\infty} (-1)^{(i+1)} \frac{2}{(i\pi)^{2}} \cos(i\pi\xi) \exp[-\tau(i\pi)^{2}]$ (3.b)

After the heating period, problem (1) becomes homogeneous with initial temperature distribution given by equation (3.a) for $t = t_h$. Hence, it can easily be solved by separation of variables (Ozisik, 1993). Since the initial condition at $t = t_h$ obtained from equation (3.a) is a superposition of three one-dimensional solutions, such is also the case for the solution for $t > t_h$. The temperature field for $t > t_h$ is given by

$$T(x, y, z, t) = \frac{\overline{q}_1}{a} \theta_2(x, t, k_1) + \frac{\overline{q}_2}{b} \theta_2(y, t, k_2) + \frac{\overline{q}_3}{c} \theta_2(z, t, k_3)$$
(4.a)
where

$$\theta_{2}(\xi, t, k_{j}) = t_{h} + 2\sum_{i=1}^{\infty} \frac{(-1)^{i} \cos(i\pi\xi) \exp[-k_{j}(t-t_{h})(i\pi)^{2}] \{1 - \exp[-k_{j}(i\pi)^{2}t_{h}]\}}{k_{j}(i\pi)^{2}}$$
(4.b)

INVERSE PROBLEM

For the *inverse problem* considered here, the thermal conductivity components k_1 , k_2 and k_3 are regarded as unknown, while the other quantities appearing in the formulation of the direct problem described above are assumed to be known with high degree of accuracy.

For the estimation of the vector of unknown parameters $\mathbf{P}^{T} = [k_1, k_2, k_3]$, we assume available the transient readings of M temperature sensors. Since it is desirable to have a nonintrusive experiment, we consider the sensors to be located at the insulated surfaces x = 0, y = 0 and z = 0. We note that the temperature measurements may contain random errors. Such errors are assumed here to be additive, uncorrelated, and normally distributed with a zero mean and a known constant standard-deviation σ (Beck and Arnold, 1977). Therefore, the solution of the present parameter estimation problem can be obtained through the minimization of the ordinary least-squares norm

$$S(\mathbf{P}) = [\mathbf{Y} - \mathbf{T}(\mathbf{P})]^T [\mathbf{Y} - \mathbf{T}(\mathbf{P})]$$
(5)

-

where

$$\left[\mathbf{Y}-\mathbf{T}(\mathbf{P})\right]^{T} = \left[\vec{Y}_{1}-\vec{T}_{1}(\mathbf{P}), \vec{Y}_{2}-\vec{T}_{2}(\mathbf{P}), \cdots, \vec{Y}_{I}-\vec{T}_{I}(\mathbf{P})\right] \quad (6.a)$$

and each element $[\vec{Y}_i - \vec{T}_i(\mathbf{P})]$ is a row vector of length equal to the number of sensors M, that is,

$$[\vec{Y}_{i} - \vec{T}_{i}(\mathbf{P})] = [Y_{i1} - T_{i1}(\mathbf{P}), Y_{i2} - T_{i2}(\mathbf{P}), \cdots, Y_{iM} - T_{iM}(\mathbf{P})]$$

for $i = 1, ..., I$ (6.b)

We note that Y_{im} and $T_{im}(\mathbf{P})$ are the measured and estimated temperatures, respectively, for time t_i , i=1,...,I, and for the sensor m, m=1,...,M. The estimated temperatures are obtained from the solution of the direct problem given by equations (3,4), by using the current available estimate for the vector of unknown parameters $\mathbf{P}^{\mathrm{T}} = [k_1, k_2, k_3]$.

The methods considered in this paper for the minimization of the least squares norm (5) make use of the *sensitivity matrix*. For the present case, involving multiple measurements to estimate the vector of unknown parameters $\mathbf{P}^{\mathrm{T}} = [k_1, k_2, k_3]$, the sensitivity matrix is defined as

$$\mathbf{J}(\mathbf{P}) \equiv \begin{bmatrix} \frac{\partial \mathbf{T}_{1}^{T}}{\partial \mathbf{P}} \end{bmatrix}^{T} = \begin{bmatrix} \frac{\partial \vec{T}_{1}^{T}}{\partial k_{1}} & \frac{\partial \vec{T}_{1}^{T}}{\partial k_{2}} & \frac{\partial \vec{T}_{1}^{T}}{\partial k_{3}} \\ \frac{\partial \vec{T}_{2}^{T}}{\partial k_{1}} & \frac{\partial \vec{T}_{2}^{T}}{\partial k_{2}} & \frac{\partial \vec{T}_{2}^{T}}{\partial k_{3}} \\ \vdots & \vdots & \vdots \\ \frac{\partial \vec{T}_{1}^{T}}{\partial k_{1}} & \frac{\partial \vec{T}_{1}^{T}}{\partial k_{2}} & \frac{\partial \vec{T}_{1}^{T}}{\partial k_{3}} \end{bmatrix}$$
(7)

The elements of the sensitivity matrix are denoted *Sensitivity Coefficients*. Due to the analytical nature of the solution of the direct problem given by equations (3,4), we can also obtain analytic expressions for the sensitivity coefficients. Since the solution of the direct problem is obtained as a superposition of one-dimensional solutions, we note that the sensitivity coefficient with respect to k_1 is a function of x, but not of y and z. The expressions for the sensitivity coefficients with respect to k_1 are obtained as

$$J_{1} = -\frac{\overline{q}_{1} a}{k_{1}^{2}} \theta_{1} \left(\frac{x}{a}, \frac{k_{1} t}{a^{2}} \right) + \frac{\overline{q}_{1} t}{k_{1} a} \left\{ 1 - 2 \sum_{i=1}^{\infty} (-1)^{1+i} \cos\left(\frac{i \pi x}{a}\right) \exp\left[\frac{(-k_{1} t)(i \pi)^{2}}{a^{2}}\right] \right\}$$
(8.a)
for $0 < t \le t_{h}$

and

$$J_{1} = \frac{2 \overline{q}_{1}}{a k_{1}^{2}} \sum_{i=1}^{\infty} \frac{(-1)^{i} \cos(i \pi x) \exp[-k_{1} (i \pi)^{2} t]}{(i \pi)^{2}} \\ \{k_{1} (i \pi)^{2} \{\exp[k_{1} (i \pi)^{2} t_{h}](t - t_{h}) - t\} + \text{ for } t > t_{h} \\ + \exp[k_{1} (i \pi)^{2} t_{h}] - 1\}$$
(8.b)

and analogous expressions can be obtained for the sensitivity coefficients J_2 and J_3 with respect to k_2 and k_3 , respectively. We note that the present estimation problem is non-linear, since the sensitivity coefficients are functions of the unknown parameters.

METHODS OF SOLUTION

For the minimization of the least squares norm (5), we consider here the *Levenberg-Marquardt Method* (Levenberg, 1944, Marquardt, 1963, Beck and Arnold, 1977, Mejias et al, 1999, Ozisik and Orlande, 1999) and the *Conjugate Gradient Method* versions of *Fletcher-Reeves*, *Polak-Ribiere*, *Powell-Beale* and *Hestenes-Stieffel* (Alifanov, 1994, Daniel, 1971, Ozisik and Orlande, 1999, Powell, 1977, Hestenes and Stiefel, 1952, Fletcher and Reeves, 1964, Colaço and Orlande, 1999). These methods can be suitably arranged in iterative procedures of the form

$$\mathbf{P}^{k+1} = \mathbf{P}^k + \Delta \mathbf{P}^k \tag{9}$$

where $\Delta \mathbf{P}^k$ is the increment in the vector of unknown parameters at iteration *k*. The computation of $\Delta \mathbf{P}^k$ for each of the methods considered here are addressed next.

1. Levenberg-Marquardt Method

The so-called *Levenberg-Marquardt Method* was first derived by Levenberg (1944) by modifying the ordinary least squares norm. Later Marquardt (1963) derived basically the same technique by using a different approach. Marquardt's intention was to obtain a method that would tend to the Gauss method in the neighborhood of the minimum of the ordinary least squares norm, and would tend to the steepest descent method in the neighborhood of the initial guess used for the iterative procedure.

The increment $\Delta \mathbf{P}^k$ for the Levenberg-Marquardt Method can be written as

$$\Delta \mathbf{P}^{k} = [(\mathbf{J}^{k})^{T} \mathbf{J}^{k} + \mu^{k} \Omega^{k}]^{-1} (\mathbf{J}^{k})^{T} [\mathbf{Y} - \mathbf{T}(\mathbf{P}^{k})]$$
(10)

where μ^{k} is a positive scalar named *damping parameter*, and $\mathbf{\Omega}^{k}$ is a *diagonal matrix*.

The purpose of the matrix term $\mu^k \mathbf{\Omega}^k$ in equation (10) 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, since the problem is generally ill-conditioned in the region around the initial guess used for the iterative procedure, which can be quite far from the exact parameters. 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 μ^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 and Arnold, 1977, Ozisik and Orlande, 1999).

The following criteria are used to stop the iterative procedure of the Levenberg-Marquardt Method:

 $S(\mathbf{P}^{k+1}) < \varepsilon_1$ (i) (11.a)

(ii)
$$| (\mathbf{J}^k)^T [\mathbf{Y} - \mathbf{T} (\mathbf{P}^k)] | < \varepsilon_2$$
 (11.b)

(iii)
$$\left\| \mathbf{P}^{k+1} - \mathbf{P}^k \right\| < \varepsilon_3$$
 (11.c)

where ε_1 , ε_2 and ε_3 are user prescribed tolerances and $\| \cdot \|$ is the vector Euclidean norm, i.e., $\|\mathbf{x}\| = (\mathbf{x}^T \mathbf{x})^{\frac{1}{2}}$, where the superscript *T* denotes transpose.

The criterion given by equation (11.a) tests if the least squares norm is sufficiently small, which is expected to be in the neighborhood of the solution for the problem. Similarly, equation (11.b) checks if the norm of the gradient of $S(\mathbf{P})$ is sufficiently small, since it is expected to vanish at the point where $S(\mathbf{P})$ is minimum. Although such a condition of vanishing gradient is also valid for maximum and saddle points of $S(\mathbf{P})$, the Levenberg-Marguardt method is very unlike to converge to such points. The last criterion given by equation (11.c) results from the fact that changes in the vector of parameters are very small when the method has converged.

Different versions of the Levenberg-Marquardt method can be found in the literature, depending on the choice of the diagonal matrix $\mathbf{\Omega}^{k}$ and on the form chosen for the variation of the damping parameter μ^k . We illustrate here the computational algorithm of the method with the matrix $\mathbf{\Omega}^{k}$ taken as

$$\Omega^{k} = diag[(\mathbf{J}^{k})^{T}\mathbf{J}^{k}]$$
(12)

Suppose that temperature measurements are given at times t, i=1,...,I. Also, suppose that an initial guess \mathbf{P}^0 is available for the vector of unknown parameters **P**. Choose a value for μ^0 , say, $\mu^0 = 0.001$ and set k = 0. Then,

- Step 1. Solve the direct heat transfer problem given by equations (1) with the available estimate \mathbf{P}^k .
- Compute $S(\mathbf{P}^k)$ from equation (5). Step 2.
- Compute the sensitivity matrix \mathbf{J}^k defined by Step 3. equation (7) and then the matrix $\mathbf{\Omega}^{k}$ given by equation (12).
- Step 4. Compute the increments for the unknown parameters by using equation (10).
- Compute the new estimate \mathbf{P}^{k+1} as Step 5. $\mathbf{P}^{k+1} = \mathbf{P}^k + \Delta \mathbf{P}^k$
- Solve now the direct problem (1) with the new estimate \mathbf{P}^{k+1} in order to find $\mathbf{T}(\mathbf{P}^{k+1})$. Then compute $S(\mathbf{P}^{k+1})$, as defined by equation (5). If $S(\mathbf{P}^{k+1}) \ge S(\mathbf{P}^{k})$, replace μ^{k} by $10\mu^{k}$ and return to Step 6.
- Step 7.
- step 4. If $S(\mathbf{P}^{k+1}) \leq S(\mathbf{P}^{k})$, accept the new estimate \mathbf{P}^{k+1} and replace μ^{k} by $0.1\mu^{k}$. Step 8.

Step 9. Check the stopping criteria given by equations (11.a-c). Stop the iterative procedure if any of them is satisfied; otherwise, replace k by k+1 and return to step 3.

In another version of the Levenberg-Marquardt method due to Moré(1977) the matrix $\mathbf{\Omega}^{k}$ is taken as the *identity matrix* and the damping parameter μ^{k} is chosen based on the so-called trust region algorithm. The subroutines of the IMSL (1987) are based on this version of the Levenberg-Marquardt Method.

2. Conjugate Gradient Method

The Conjugate Gradient Method is a straightforward and powerful iterative technique for solving inverse problems of parameter estimation. In the iterative procedure of the Conjugate Gradient Method, at each iteration a suitable step size is taken along a direction of descent in order to minimize the objective function. The direction of descent is obtained as a linear combination of the negative gradient direction at the current iteration with directions of descent from previous iterations. The Conjugate Gradient Method with an appropriate stopping criterion belongs to the class of iterative regularization techniques, in which the number of iterations is chosen so that stable solutions are obtained for the inverse problem (Alifanov, 1994, Ozisik and Orlande, 1999).

The increment in the vector of unknown parameters at each iteration of the conjugate gradient method is given by

$$\Delta \mathbf{P}^{k} = \boldsymbol{\beta}^{k} \mathbf{d}^{k} \tag{14}$$

The search step size β^k is obtained by minimizing the objective function given by equation (5) with respect to β^k . By using a first-order Taylor series approximation for the estimated temperatures, the following expression results for the search step size(Ozisik and Orlande, 1999):

$$\boldsymbol{\beta}^{k} = \frac{[\mathbf{J}^{k}\mathbf{d}^{k}]^{T}[\mathbf{Y} - \mathbf{T}(\mathbf{P}^{k})]}{[\mathbf{J}^{k}\mathbf{d}^{k}]^{T}[\mathbf{J}^{k}\mathbf{d}^{k}]}$$
(15)

The *direction of descent* \mathbf{d}^{k} is given in the following general form

$$\mathbf{d}^{k} = -\nabla S(\mathbf{P}^{k}) + \gamma^{k} \mathbf{d}^{k-1} + \boldsymbol{\psi}^{k} \mathbf{d}^{q}$$
(16)

where γ^k and ψ^k are conjugation coefficients and $\nabla S(\mathbf{P}^k)$ is the gradient vector given by

$$\nabla S(\mathbf{P}^{k}) = -2(\mathbf{J}^{k})^{T} [\mathbf{Y} - \mathbf{T}(\mathbf{P}^{k})]$$
(17)

The superscript q in equation (16) denotes the iteration number where a *restarting strategy* is applied to the iterative procedure of the conjugate gradient method. Restarting strategies were suggested for the conjugate gradient method of parameter estimation in order to improve its convergence rate (Powell, 1977).

Different versions of the Conjugate Gradient Method can be found in the literature depending on the form used for the

(13)

computation of the direction of descent given by equation (16) (Alifanov, 1994, Daniel, 1971, Ozisik and Orlande, 1999, Powell, 1977, Hestenes and Stiefel, 1952, Fletcher and Reeves, 1964, Colaço and Orlande, 1999). In the *Fletcher-Reeves* version, the conjugation coefficients γ^k and ψ^k are obtained from the following expressions

$$\gamma^{k} = \frac{\left[\nabla S(\mathbf{P}^{k})\right]^{\mathrm{T}} \left[\nabla S(\mathbf{P}^{k})\right]}{\left[\nabla S(\mathbf{P}^{k-1})\right]^{\mathrm{T}} \left[\nabla S(\mathbf{P}^{k-1})\right]} \quad \text{with } \gamma^{0} = 0 \text{ for } \mathbf{k} = 0 \qquad (18.a)$$

$$\psi^k = 0$$
 for $k = 0, 1, 2, ...$ (18.b)

In the *Polak-Ribiere* version of the Conjugate Gradient Method the conjugation coefficients are given by

$$\gamma^{k} = \frac{\left[\nabla S(\mathbf{P}^{k})\right]^{\mathrm{T}} \left[\nabla S(\mathbf{P}^{k}) \cdot \nabla S(\mathbf{P}^{k-1})\right]}{\left[\nabla S(\mathbf{P}^{k-1})\right]^{\mathrm{T}} \left[\nabla S(\mathbf{P}^{k-1})\right]} \text{ with } \gamma^{0} = 0 \text{ for } k=0 \quad (19.a)$$

$$\psi^k = 0$$
 for $k = 0, 1, 2, ...$ (19.b)

For the *Hestenes-Stiefel* version of the Conjugate Gradient Method we have

$$\gamma^{k} = \frac{\left[\nabla S(\mathbf{P}^{k})\right]^{\mathrm{T}} \left[\nabla S(\mathbf{P}^{k}) - \nabla S(\mathbf{P}^{k-1})\right]}{\left[\mathbf{d}^{k-1}\right]^{\mathrm{T}} \left[\nabla S(\mathbf{P}^{k}) - \nabla S(\mathbf{P}^{k-1})\right]} \text{ with } \gamma^{0} = 0 \text{ for } k=0$$
(20.a)

$$\psi^k = 0$$
 for $k = 0, 1, 2, ...$ (20.b)

Powell(1977) suggested the following expressions for the conjugation coefficients, which gives the so-called *Powell-Beale's* version of the conjugate gradient method

$$\gamma^{k} = \frac{\left[\nabla S(\mathbf{P}^{k})\right]^{T} \left[\nabla S(\mathbf{P}^{k}) - \nabla S(\mathbf{P}^{k-1})\right]}{\left[\mathbf{d}^{k-1}\right]^{T} \left[\nabla S(\mathbf{P}^{k}) - \nabla S(\mathbf{P}^{k-1})\right]} \text{ with } \gamma^{0} = 0 \text{ for } k=0 \quad (21.a)$$
$$\psi^{k} = \frac{\left[\nabla S(\mathbf{P}^{k})\right]^{T} \left[\nabla S(\mathbf{P}^{q+1}) - \nabla S(\mathbf{P}^{q})\right]}{\left[\mathbf{d}^{q}\right]^{T} \left[\nabla S(\mathbf{P}^{q+1}) - \nabla S(\mathbf{P}^{q})\right]} \text{ with } \psi^{0} = 0 \quad (21.b)$$
for $k = 0$

In accordance with Powell(1977), the application of the conjugate gradient method with the conjugation coefficients given by equations (21) requires restarting when gradients at successive iterations tend to be non-orthogonal (which is a measure of the local non-linearity of the problem) and when the direction of descent is not sufficiently downhill. Restarting is performed by making $\psi^{k} = 0$ in equation (16).

The non-orthogonality of gradients at successive iterations is tested by using:

$$ABS([\nabla S(\mathbf{P}^{k-1})]^{\mathrm{T}}[\nabla S(\mathbf{P}^{k})]) \ge 0.2[\nabla S(\mathbf{P}^{k})]^{\mathrm{T}}[\nabla S(\mathbf{P}^{k})] \quad (22.a)$$

where ABS (.) denotes the absolute value.

A non-sufficiently downhill direction of descent (i.e., the angle between the direction of descent and the negative gradient direction is too large) is identified if either of the following inequalities are satisfied:

$$[\mathbf{d}^{k}]^{\mathrm{T}}[\nabla S(\mathbf{P}^{k})] \leq -1.2[\nabla S(\mathbf{P}^{k})]^{\mathrm{T}}[\nabla S(\mathbf{P}^{k})]$$
(22.b)

or

$$[\mathbf{d}^{k}]^{\mathrm{T}}[\nabla S(\mathbf{P}^{k})] \ge -0.8[\nabla S(\mathbf{P}^{k})]^{\mathrm{T}}[\nabla S(\mathbf{P}^{k})]$$
(22.c)

In Powell-Beale's version of the conjugate gradient method, the direction of descent given by equation (16) is computed in accordance with the following algorithm for $k \ge 1$:

<u>STEP 1:</u> Test the inequality (22.a). If it is true set q = k-1.

- <u>STEP 2:</u> Compute γ^k with equation (21.a).
- <u>STEP 3</u>: If k = q+1 set $\psi^k = 0$. If $k \neq q+1$ compute ψ^k with equation (21.b).
- <u>STEP 4:</u> Compute the search direction $\mathbf{d}^{k}(X,Y,\tau)$ with equation (16).
- <u>STEP 5:</u> If $k \neq q+1$ test the inequalities (22.b,c). If either one of them is satisfied set q = k-1 and $\psi^{k}=0$. Then recompute the search direction with equation (16).

The iterative procedure given by equations (9,14-21) does not provide the conjugate gradient method with the stabilization necessary for the minimization of the objective function (5) to be classified as well-posed. Therefore, as the estimated temperatures approach the measured temperatures containing errors, during the minimization of the function (5), large oscillations may appear in the inverse problem solution. However, the conjugate gradient method may become wellposed if the *Discrepancy Principle* (Alifanov, 1994) is used to stop the iterative procedure.

In the discrepancy principle, the iterative procedure is stopped when the following criterion is satisfied

$$S(\mathbf{P}^{k+1}) < \varepsilon \tag{23}$$

where the value of the tolerance ε is chosen so that sufficiently stable solutions are obtained. In this case, we stop the iterative procedure when the residuals between measured and estimated temperatures are of the same order of magnitude of the measurement errors, that is,

$$|Y_{im} - T_{im}| \approx \sigma \tag{24}$$

where σ is the standard deviation of the measurement errors, which is supposed constant and known. By substituting equation (24) into equation (5), we obtain ε as

$$\varepsilon = I M \sigma^2 \tag{25}$$

If the measurements are regarded as errorless, the tolerance ε can be chosen as a sufficiently small number, since the expected minimum value for the objective function (5) is zero.

The iterative procedure of the conjugate gradient method can be suitably arranged in the following computational algorithm.

Suppose that temperature measurements and an initial guess \mathbf{P}^0 is available for the vector of unknown parameters \mathbf{P} . Set k = 0 and then

Step 1. Solve the direct heat transfer problem (1) by using the available estimate \mathbf{P}^k and obtain the vector of estimated temperatures $\mathbf{T}(\mathbf{P}^k)$.

- **Step 2.** Check the stopping criterion given by equation (23). Continue if not satisfied.
- **Step 3.** Compute the sensitivity matrix \mathbf{J}^k defined by equation (7).
- **Step 4.** Compute the gradient direction $\nabla S(\mathbf{P}^k)$ from equation (17) and then the conjugation coefficients from equations (18), (19), (20) or (21). Note that Powell-Beale's version requires restarting if any of the inequalities (22.a-c) are satisfied.
- **Step 5.** Compute the direction of descent \mathbf{d}^k by using equation (16).
- **Step 6.** Compute the search step size β^k from equation (15).
- **Step 7.** Compute the increment $\Delta \mathbf{P}^k$ with equation (14) and then the new estimate \mathbf{P}^{k+1} with equation (9). Replace *k* by *k*+1 and return to step 1.

RESULTS AND DISCUSSIONS

For the results presented below, we assumed the solid with unknown thermal conductivities to be available in the form of a cube, so that a = b = c = 1. Also, the heat fluxes applied on the boundaries x = a = 1, y = b = 1 and z = c = 1 were assumed to be of equal magnitude during the heating period $0 < t \le t_h$, so that $\overline{q}_i = 1$ in equation (2), for j = 1,2,3. Different experimental variables, such as the number and locations of sensors, heating time and final time, optimally chosen by Mejias et al (1999), were used here for the analysis of test-cases involving different values for the unknown thermal conductivity components. The test-cases examined here are summarized in table 1, together with their respective optimal values of heating and final times. The readings of three sensors (M=3) located at the positions (0,0.9,0.9), (0.9,0,0.9) and (0.9,0.9,0) were used for the estimation of the unknown thermal conductivity components. One hundred simulated measurements per sensor, containing additive, uncorrelated and normally distributed errors with zero mean and constant standard-deviation, were assumed available for the estimation procedure.

The computational algorithms presented above for the Levenberg-Marquardt method, as well as for the different versions of the conjugate gradient method, were programmed in FORTRAN 90 and applied to the estimation of the parameters shown in table 1, by using simulated measurements with standard deviations of $\sigma = 0$ (errorless measurements) and $\sigma = 0.01T_{max}$, where T_{max} is the maximum measured temperature. For the comparison presented below, we also considered the IMSL (1987) version of the Levenberg-Marquardt method in the form of the subroutine DBCLSJ. Upper and lower limits for the unknown parameters, required by such subroutine, were taken as 10^{-3} and 10^4 , respectively. The same limits were also considered in the implementation of the other estimation techniques. Table 2 summarizes the techniques used in the present paper.

Tables 3 to 5 present the results obtained for the CPU time, average rate of reduction of the objective function with

respect to the number of iterations (r) and RMS error (e_{RMS}), obtained with each of the techniques summarized in table 2, for the test-cases 1 to 3, respectively. The computations were performed in a Pentium 100 MHz, under the Fortran PowerStation platform. The results presented in tables 3 and 4 were obtained with an initial guess $P^0=[0.1,0.1,0.1]$ for the unknown parameters, while an initial guess of $P^0=[0.5,0.5,0.5]$ was required for convergence of any of the methods for test-case 3 (table 5). For those cases involving simulated measurements with random errors, the results shown in tables 3-5 were averaged over 10 different runs, in order to reduce the effects of the random number generator utilized.

The average rates of reduction of the objective function (r) were obtained from the following approximation for the variation of $S(\mathbf{P})$ with the number of iterations (N):

$$S(\mathbf{P}) = CN^{-r} \tag{26}$$

where C is a constant depending on the data.

The RMS errors were computed as

$$e_{RMS} = \sqrt{\frac{1}{3} \sum_{j=1}^{3} (k_{ex,j} - k_{est,j})^2}$$
(27)

where the subscripts ex and est refer to the exact and estimated parameters, respectively.

Table.1.	Test-cases	with 1	respective	heating	and	final ti	mes.

Case	Exact Parameters			t_h	t_f
	k_1	k_2	k_3		
1	1	1.5	2	0.2	0.28
2	1	2	3	0.15	0.2
3	1	15	15	0.03	0.05

Table 2. Techniques used for the estimation of the unknown parameters.

Technique	Method	Version
1A	Levenberg-Marquardt	This paper
1B	Levenberg-Marquardt	IMSL
2A	Conjugate Gradient Method	Fletcher-Reeves
2B	Conjugate Gradient Method	Polak-Ribiere
2C	Conjugate Gradient Method	Hestenes-Stiefel
2D	Conjugate Gradient Method	Powell-Beale

The tolerances for the stopping criteria of technique 1A were taken as $\varepsilon_1 = \varepsilon_2 = \varepsilon_3 = 10^{-15}$ in equations (11.a-c), for cases involving errorless measurements, as well as measurements with random errors. For those cases involving errorless measurements, the tolerances for the stopping criterion of techniques 2A-D were taken as $\varepsilon = 10^{-15}$ in equation (23). For those cases involving measurements with random errors, such tolerances for techniques 2A-D were obtained from

equation(25) based on the discrepancy principle. We note that the tolerances for the stopping criteria of technique 1B were set internally by the subroutine DBCLSJ of the IMSL (1987).

Table 3. Results for test-case 1

Technique	σ	CPU time (s)	r	e _{RMS}
1.4	0.00	2.4	18	0.00
IA	0.01T _{max}	4.0	4	0.01
1D	0.00	2.5	18	0.00
ID	$0.01T_{max}$	2.6	4	0.01
2.4	0.00	4.7	14	0.00
ZA	$0.01T_{max}$	5.5	2	0.01
2B	0.00	4.7	14	0.00
	0.01T _{max}	4.2	3	0.02
2C	0.00	6.3	13	0.00
	$0.01T_{max}$	6.9	2	0.01
2D	0.00	4.4	10	0.00
	0.01T _{max}	4.9	3	0.01

Table 4. Results for test-case 2

Technique	σ	CPU time (s)	r	e _{RMS}
1 4	0.00	2.7	22	0.00
IA	$0.01T_{max}$	4.3	4	0.01
1D	0.00	3.1	31	0.00
ID	$0.01T_{max}$	3.0	4	0.02
2A	0.00	7.1	12	0.00
	0.01T _{max}	6.6	3	0.02
2B	0.00	4.9	13	0.00
	$0.01T_{max}$	6.0	3	0.02
2C	0.00	6.9	14	0.00
	0.01T _{max}	6.0	3	0.02
2D	0.00	5.2	14	0.00
	0.01T _{max}	4.9	3	0.03

Table 5. Results for test-case 3

Technique	σ	CPU time (s)	r	e _{RMS}
1.4	0.00	3.2	23	0.00
IA	0.01T _{max}	5.1	3	0.12
1D	0.00	3.6	27	0.00
ID	0.01T _{max}	3.4	4	0.13
2.4	0.00	5.6	12	0.00
ZA	$0.01T_{max}$	8.8	2	0.17
2B	0.00	5.4	10	0.00
	0.01T _{max}	9.7	2	0.12
2C	0.00	5.8	9	0.00
	0.01T _{max}	17.9	2	0.38
2D	0.00	5.8	9	0.00
	0.01T _{max}	12.6	3	0.12

Let us consider first in the analysis of tables 3-5 the cases involving errorless measurements ($\sigma = 0$). Tables 3-5 show that all techniques were able to estimate exactly the three different sets of unknown parameters examined, resulting in $e_{RMS} = 0.00$. The highest rates of reduction of the objective function were obtained with the Levenberg-Marquardt method and, for such method, technique 1B had a better performance than technique 1A, except for test-case 1 (table 3) where both techniques were equivalent. The rates of reduction of the objective function were of the order of 20 (minimum of 18) or higher for the Levenberg-Marquardt method, while such rates were of the order of 10 (maximum of 14) for the conjugate gradient method. The CPU times were generally smaller for the Levenberg-Marquardt method (techniques 1A and 1B) than for the conjugate gradient method (techniques 2A-2D).

Tables 3-5 show a strong reduction of the rate of reduction of the objective function when measurements with random errors were used in the analysis, instead of errorless measurements. Such a behavior was also observed in a nonlinear function estimation problem (Colaço and Orlande, 1999). As for the cases with errorless measurements, the Levenberg-Marquardt method had a performance superior than that of the conjugate gradient method in terms of CPU time and rate of reduction of the objective function, for the cases with measurements with random errors. All techniques resulted in accurate estimates for the unknown parameters when measurements with random errors were used in the analysis; but relative high RMS errors were noticed with techniques 2A and 2C for test-case 3.

We note that the use of the discrepancy principle was not required to provide the Levenberg-Marquardt method with the regularization necessary to obtain stable solutions for those cases involving measurements with random errors. The computational experiments revealed that the Levenberg-Marquardt method, through its automatic control of the damping parameter μ^k , reduced drastically the increment in the vector of estimated parameters, at the iteration where the measurement errors started to cause instabilities on the inverse problem solution. The iterative procedure of the Levenberg-Marquardt method was then stopped by the criterion given by equation (11.c). For some cases we also noticed that the iterative procedure of the Levenberg-Marquardt method was stopped by the criterion (11.b) when measurements with random errors were used in the analysis, that is, the norm of gradient vector became very small.

Table 6 is prepared to illustrate the effect of the initial guess for the parameters, i.e., \mathbf{P}^0 , over the rate of reduction of the objective function. Three different initial guesses were considered for test-case 1, by using errorless measurements in the analysis. Table 6 shows that, although the rate of reduction jumped to 24 for technique 1A for the initial guess $\mathbf{P}^0=[3,3,3]$, the values of such rate were insensitive to the three initial guesses, with all techniques examined in this paper. We note that techniques 2A-D, based on the conjugate gradient method, did not converge to the exact parameters for initial guesses larger than $\mathbf{P}^0 = [3,3,3]$. On the other hand, techniques 1A and 1B, based on the Levenberg-Marquardt method, were able to converge to the exact parameters even with initial guesses as large as $\mathbf{P}^0 = [10,10,10]$.

Technique	r				
	$\mathbf{P}^{0} = [0.1, 0.1, 0.1]$	$\mathbf{P}^{0}=[1,1,1]$	$\mathbf{P}^{0}=[3,3,3]$		
1A	18	16	24		
1B	18	16	18		
2A	14	12	11		
2B	14	13	14		
2C	13	13	14		
2D	10	13	12		

Table 6. Effect of the initial guess on the rate of reduction of the objective function.

CONCLUSIONS

In this paper we compared 6 different parameter estimation techniques, based on the Levenberg-Marquardt method and on the conjugate gradient method, for the identification of the three thermal conductivity components of orthotropic solids. The techniques were compared in terms of rate of reduction of the objective function, CPU time and accuracy of the estimated parameters.

The foregoing analysis reveals that, besides having the highest rates of reduction of the objective function, the use of the Levenberg-Marquardt method also resulted in the smallest CPU times and in the smallest RMS errors of the estimated parameters. Such method was able to converge to the exact parameters even for initial guesses quite far from the exact values. Hence, the Levenberg-Marquardt method appears to be the best, among those tested, for the estimation of the three thermal conductivity components of orthotropic solids.

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