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Identification of the Thermal Conductivity and Heat Capacity in Unsteady Nonlinear Heat Conduction Problems Using the Boundary Element Method

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In this study the inverse problem of the identification of temperature dependent thermal properties of a heat conducting body is investigated. The solution of the corresponding direct problem is obtained using a time marching boundary element method (BEM), which allows, without any need of interpolation and solution domain discretisation, efficient and accurate evaluation of the temperature everywhere inside the space–time dependent domain. Since the inverse problem, which requires the determination of the thermal conductivity and heat capacity from a finite set of temperature measurements taken inside the body, possesses poor uniqueness features, additional information is achieved by assuming that the thermal properties belong to a set of polynomials. Thus the inverse problem reduces to a parameter system estimation problem which is solved using the nonlinear least-squares method. Convergent and stable numerical results are obtained for the finite set of parameters which characterise the thermal properties for various test examples. Once the thermal properties are accurately obtained then the BEM determines automatically the temperature inside the solution domain and the remaining unspecified boundary values and the numerically obtained results show good agreement with the corresponding analytical solutions. © 1996 Academic Press, Inc.

1. INTRODUCTION

Inverse problems in heat conduction have been the point of interest for many researchers in recent years. The determination of the unknown temperature and heat flux at an inaccessible portion of the boundary, i.e. the inverse heat conduction problem (IHCP) (see [1]) and the determination of the unknown initial temperature, i.e., the backward heat conduction problem (BHCP) (see [2, 3]) are examples of typical boundary inverse problems which arise when analysing a heat conducting material. Another type of inverse problem in heat conduction requires the estimation of the thermal properties and/or heat source time, spatially and/or temperature dependent, i.e., the identification heat conduction problem (IDHCP) (see [4–8]). In these inverse formulations the determination of the boundary or coefficient unknowns is obtained provided that additional boundary and/or interior temperature measurements are available. Steady or transient, linear or nonlinear heat conduction equations with linear and/or nonlinear boundary conditions can be formulated for the treatment of all these problems. However, it should be said that simultaneous requests resulting from combining these inverse problems are yet to be investigated.

Inverse problems are more difficult than their corresponding direct formulated problems because they are ill-posed; i.e., either existence, uniqueness, or continuous dependence upon the data (stability) are violated. In general, both the IHCP and BHCP violate stability when uniqueness is satisfied, whilst the IDHCP is more difficult since the uniqueness problem has to be addressed.

It is the purpose of this study to investigate one of the identification problems which requires the simultaneous estimation of the thermal conductivity and the heat capacity, which are temperature dependent, from boundary and initial data and additional interior temperature measurements. Also, the unknown temperature solution and the remaining unspecified boundary values are required to be determined.

Reports of analysis of inverse, nonlinear IDHCP are limited in the literature. Theoretical studies, both in steady and unsteady, linear or nonlinear cases have been investigated in [9–11]. Numerically, the first step in the inverse analysis is the development of the solution of the corresponding direct problem and previous works on the subject (see [7, 12]) have used finite differences. However, the identification of the thermal conductivity temperature dependence has been investigated using the BEM in [8] only for the steady case and it is the purpose of this study to investigate the unsteady nonlinear identification situation. The advantages of the BEM, in comparison with finite-difference or finite element methods, are that the BEM does not require any solution domain discretisation and, in addition, no need of interpolation is required when evaluating the interior estimated temperature values. Furthermore, the BEM gives in a straightforward manner both the remaining unspecified boundary values and the temperature inside the solution domain. All these advantages,

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which result in savings in the computational time and storage requirements, are important in the inverse analysis as the corresponding solution of the direct problem should be used many times, iteratively. Also, the principle of the application of the BEM is not affected by the type of boundary condition, as is the situation, for example, with the finite-difference scheme adopted in [12] which uses different implementations for Neumann and Dirichlet problems in order to ensure the stability of the method. Finally, as the purpose of this study is a first attempt to introduce the BEM for solving the nonlinear transient IDHCP, for simplicity only the one-dimensional, time-dependent case is investigated, although it should be noted that the extension of the method to higher dimensions is, in principle, straightforward and is the subject of ongoing research by the authors. A review of the BEM, as applied to direct linear and nonlinear heat conduction problems with linear or nonlinear boundary conditions, can be found in [13].

By using the Kirchhoff transformation, the governing heat conduction equation reformulates into a useful nonlinear form involving the temperature dependent thermal diffusivity coefficient which is solved using a boundary element time marching technique. Over each small time step the resulting nonlinear partial differential equation is linearised by assuming that the variation of the thermal diffusivity with temperature is usually not strong, and it is taken to be a constant which is its average mean value at the beginning of each time step. Although this assumption may appear somewhat strong, in practice, many heat conducting materials possess a weak dependence of the thermal diffusivity on the temperature; see [14]. In addition, although a theoretical investigation of this approximation is deferred to a future work, the present study also investigates numerically how the BEM performs when the problem is strongly nonlinear. Finally, it should be noted that a more general boundary element approach for solving heat transfer problems is the dual reciprocity BEM (see, for example, [15]), but its implementation in the inverse analysis of the identification process has not been yet performed.

In the inverse analysis, the thermal properties are not known and therefore the BEM is employed with an iterative procedure, with the termination criterion being the minimization of the nonlinear least-squares functional. Further, in order to render a unique solution, the function estimation problem is reformulated as a parameter estimation problem by assuming that the thermal properties belong to a set of polynomials. In addition, physical positive constraints and fixing conditions are imposed to the solution which minimizes the functional. Once the thermal properties are accurately estimated, the BEM gives automatically, at the final iterate, the temperature everywhere in the solution domain and the remaining unspecified boundary values.

The inversion method has been applied to various test examples which involve constant, linear or quadratic representation of the thermal properties and the numerical results show good agreement with the analytical solutions.

2. FORMULATION OF THE PROBLEM

The mathematical formulation of the one-dimensional, transient, nonlinear heat conduction problem in a slab geometry considered in this study, in nondimensional form, is given by

$$\rho(T)c_p(T)\frac{\partial T(x,t)}{\partial t} = \frac{\partial}{\partial x}\left(k(T)\frac{\partial T(x,t)}{\partial x}\right), \quad (x,t) \in (0,1) \times (0,1] \tag{1a}$$

$$T(x,t) = f_0(t) \quad \text{at } x = 0, t \in (0,1] \tag{1b}$$

$$T(x,t) = f_1(t) \quad \text{at } x = 1, t \in (0,1] \tag{1c}$$

$$T(x,t) = T_0(x) \quad \text{for } t = 0, x \in [0,1], \tag{1d}$$

where T is the temperature, $k(T)$ is the thermal conductivity, $\rho(T)$ is the density, $c_p(T)$ is the specific heat, $C(T) = \rho(T)c_p(T)$ is the heat capacity, $f_0(t)$, $f_1(t)$, and $T_0(x)$ are known functions and it is assumed there is no heat generation inside the solution domain. In expressions (1) the distance, time, heat capacity, and thermal conductivity have been nondimensionalised with respect to l (the length of the slab), t_f (a final time of interest during which a specific practical heat conduction experiment is performed), and C_r and k_r (reference values), respectively. Further, we assume that a temperature sensor is installed at an arbitrary spatial position $x = d \in (0,1)$ and temperature measurements $T^{(m)}(t)$ are recorded in time, namely,

$$T(x, t) = T^{(m)}(t) \quad \text{at } x = d, t \in (0,1]. \tag{2}$$

Then, the IDHCP requires the determination of thermal properties $C(T)$ and $k(T)$ and the temperature solution T.

The first step in the inverse analysis is to develop the corresponding direct solution for the problem (1), and for this purpose the BEM is briefly introduced in the next section. A suitable form for using the BEM consists in applying the Kirchhoff transformation which can be expressed as (see, for example, [16])

$$\Psi(T) = \int_0^T k(T)\,dT. \tag{3}$$

Denoting

$$\psi(x, t) = \Psi(T(x, t)), \quad (x, t) \in [0,1] \times [0,1], \tag{4}$$

then Eqs. (1a)–(1d) in the new variable ψ can be written as

$$\frac{\partial\psi(x,t)}{\partial t} = a(T(x,t))\frac{\partial^2\psi(x,t)}{\partial x^2}, \quad (x,t) \in (0,1)\times(0,1] \tag{5a}$$

$$\psi(x,t) = \Psi(f_0(t)) \quad \text{at } x = 0, t \in (0,1] \tag{5b}$$

$$\psi(x,t) = \Psi(f_1(t)) \quad \text{at } x = 1, t \in (0,1] \tag{5c}$$

$$\psi(x,t) = \Psi(T_0(x)) \quad \text{for } t = 0, x \in [0,1], \tag{5d}$$

where

$$a(T) = \frac{k(T)}{C(T)} \tag{6}$$

is the thermal diffusivity.

3. THE BOUNDARY ELEMENT METHOD

The BEM requires only the discretisation of the boundary of the solution domain under investigation into a series of elements similar to those used in finite elements but with one degree of dimensionality less. If, in addition, a fundamental solution for the governing partial differential equation is available then the problem may be reformulated in an integral representation form involving only boundary solution domain integrals.

If the thermal diffusivity is constant, i.e., $a(T) \equiv a \equiv$ constant, then for the partial differential Eq. (5a), a fundamental solution is available (see, for example, [17]),

$$F(x,t;\xi,\tau) = \frac{1}{(4\pi a(t-\tau))^{1/2}} \exp\left(-\frac{(x-\xi)^2}{4a(t-\tau)}\right) H(t-\tau), \tag{7}$$

where H is the Heaviside function and ξ and τ are generic space and time variables, respectively.

In the case of nonconstant thermal diffusivity the use of the fundamental solution (7) should be accompanied by a time marching technique in which $a(T)$ is assumed constant at the beginning of each time step. Therefore, starting from the initial time $t_0 = 0$, over each time element $[t_{i-1}, t_i]$, i.e., time step, the value of a is taken as the mean average, namely,

$$a_i = \overline{a(T)} = \int_0^1 a(T(x, t_{i-1}))\, dx. \tag{8}$$

Previous works on the subject (see [18, 19]) also assumed that the variation with T of the function $a(T)$ is weak, i.e., the domain integrals due to the gradients of the thermal diffusivity can be neglected, and that some kind of mean value of a is employed to linearise the nonlinear Eq. (5a). Furthermore, a preliminary study performed in [20] seems to show that a representative value for the thermal diffusivity is related to a regularization effect.

Based on the approximation (8), the use of the fundamental solution (7) enables Eq. (5a) to be transformed into the integral equation for each time step $[t_{i-1}, t_i]$ (see [21]),

$$\begin{aligned}\eta(x)\,\psi(x,t) = {} & \int_{t_{i-1}}^{t_i} a_i\psi'(0,\tau)F(x,t;0,\tau)\,d\tau \\ & + \int_{t_{i-1}}^{t_i} a_i\psi'(1,\tau)F(x,t;1,\tau)\,d\tau \\ & - \int_{t_{i-1}}^{t_i} a_i\psi(0,\tau)F'(x,t;0,\tau)\,d\tau \\ & - \int_{t_{i-1}}^{t_i} a_i\psi(1,\tau)F'(x,t;1,\tau)\,d\tau \\ & + \int_0^1 \psi(y,t_{i-1})F(x,t;y,t_{i-1})\,dy,\end{aligned} \tag{9}$$

where $(x,t) \in [0,1]\times[t_{i-1}, t_i]$, primes denote differentiation with respect to the outward normal, and $\eta(x)$ is a coefficient function which is equal to 1 for $x \in (0,1)$ and 0.5 if $x \in \{0,1\}$.

A constant BEM approximation of Eq. (9), assuming that the temperature and the heat flux are constant over each time element, can be written in the form

$$\begin{aligned}\eta(x)\,\psi(x,\tilde{t}_i) = {} & \psi'(0,\tilde{t}_i)\int_{t_{i-1}}^{t_i} a_iF(x,\tilde{t}_i;0,\tau)\,d\tau \\ & + \psi'(1,\tilde{t}_i)\int_{t_{i-1}}^{t_i} a_iF(x,\tilde{t}_i;1,\tau)\,d\tau \\ & - \psi(0,\tilde{t}_i)\int_{t_{i-1}}^{t_i} a_iF'(x,\tilde{t}_i;0,\tau)\,d\tau \\ & - \psi(1,\tilde{t}_i)\int_{t_{i-1}}^{t_i} a_iF'(x,\tilde{t}_i;1,\tau)\,d\tau \\ & + \sum_{j=1}^{N_0}\psi(\tilde{y}_j,t_{i-1})\int_{y_{j-1}}^{y_j} F(x,\tilde{t}_i;y,t_{i-1})\,dy,\end{aligned} \tag{10}$$

where $\tilde{t}_i = (t_{i-1} + t_i)/2$ is the midpoint of the element $[t_{i-1}, t_i]$ and $\tilde{y}_j = (y_{j-1} + y_j)/2$, for $j = \overline{1, N_0}$, are the midpoints of the elements $[y_{j-1}, y_j]$ which are used to discretise the segment $[0,1]$ into N_0 elements. The integrals in Eq. (10) are calculated analytically; see [22]. Although the last term in Eq. (10) has resulted from discretising a space domain integral this term is evaluated analytically and, therefore, no additional computational time is required.

Since only the temperature is prescribed at each boundary point, Eq. (10) can be used to calculate the unknown boundary values for the heat flux. In order to do this, we let the point x tend to 0 and to 1, obtaining two integral equations which produce a system of two linear, algebraic equations with two unknowns. The solution of this system of equations provides the values of the transformed heat flux on the boundaries $x = 0$ and $x = 1$, namely $\psi'(0, \tilde{t}_i)$ and $\psi'(1, \tilde{t}_i)$, which then can be used in Eq. (10) for calculating the transformed temperature function ψ at any point inside the layer $[0, 1] \times [t_{i-1}, t_i]$. Once the values of ψ are obtained, the temperature T is calculated by inverting the transformation (4), namely,

$$T(x, t) = \Psi^{-1}(\psi(x, t)), \quad (x, t) \in [0, 1] \times [t_{i-1}, t_i]. \quad (11)$$

In particular, the values of ψ at $t = t_i$, namely $\psi(\tilde{y}_j, t_i)$, for $j = \overline{1, N_0}$, need to be calculated in order to provide the "initial" condition at the time t_i and to proceed to the next time step $[t_i, t_{i+1}]$. Also the corresponding values of the temperature, $T(\tilde{y}_j, t_i)$, for $j = \overline{1, N_0}$, are required in order to calculate the new constant value of the thermal diffusivity a_{i+1}, given by expression (8) at the time t_{i+1}. At this stage it should be noted that the BEM procedure over each time step has used a significant computational time only in the inversion of a 2×2 matrix. However, using the finite-difference method for the same situation requires the inversion of a $N_0 \times N_0$ sparse matrix.

Based on this time marching technique, the BEM provides the values of ψ and T at any point in the solution domain and, in particular, the calculated values of the temperature at $x = d$, $T^{(c)}(t)$, where the sensor is located, are of special interest for the inverse analysis explained in the next section. Furthermore, the BEM does not require any modification in its principle when it is applied to other types of boundary conditions or when it is extended to higher dimensional geometries.

4. IDENTIFICATION OF THE THERMAL PROPERTIES

If the thermal properties $C(T)$ and $k(T)$ are unknown then the BEM, as explained in Section 3, should be used, along with an iterative procedure. Also, if the IDHCP is linear, i.e., C and k are constant, then the BEM is exactly formulated and no further transformation (3) is needed. Initial guesses of $C(T)$ and $k(T)$ will produce a solution for the temperature at $x = d$, $T^{(c)}(t)$, which is then compared with the measured values $T^{(m)}(t)$ given by expression (4). This comparison is based on minimizing the least-squares norm $\|T^{(c)} - T^{(m)}\|^2$ which is very natural by minimizing the gap between the computed and the measured values and also guarantees the existence of the inverse solution.

In practice, only a finite set of time measurements may be available at some discrete times, t_i', for $i = \overline{1, N_T}$, namely

$$T(d, t_i') = T^{(m)}(t_i') = T_i^{(m)}, \quad i = \overline{1, N_T}. \quad (12)$$

By requiring that the continuous functions $C(T)$ and $k(T)$ be determined from only a finite set of data, as given by expression (12), will nevertheless result in a nonunique solution problem. In order to be able to achieve a unique solution the unknown thermal property functions $C(T)$ and $k(T)$ should be parameterised and thus reduce the problem from an infinite-dimensional, functional estimation problem to a finite-dimensional, parameter estimation problem. In this study, the parameterisation is performed by assuming that the functions $C(T)$ and $k(T)$ belong to a finite-dimensional space of functions $\mathbb{F}$ which is taken as the set of polynomials,

$$\mathbb{F} = \left\{ f; f(T) = \sum_{i=1}^{L} b_i T^{i-1}; L \geq 1 \right\}. \quad (13)$$

Piecewise linear or quadratic space functions may also be introduced (see [23]), but this approach will be investigated in another study.

If $C(T)$ and $k(T) \in \mathbb{F}$ then

$$C(T) = \sum_{i=1}^{L} C_i T^{i-1} \quad (14a)$$

$$k(T) = \sum_{i=1}^{L} k_i T^{i-1} \quad (14b)$$

and the least-squares norm in discretised form becomes

$$S(\mathbf{C}, \mathbf{k}) = \sum_{i=1}^{N_T} [T_i^{(m)} - T_i^{(c)}(\mathbf{C}, \mathbf{k})]^2, \quad (15)$$

where $\mathbf{C} = (C_j)$, $\mathbf{k} = (k_j)$, for $j = \overline{1, L}$, are the unknown vectors of the thermal conductivity and heat capacity, as given by expressions (14), and $T_i^{(c)}(\mathbf{C}, \mathbf{k})$ is the calculated value of the temperature at $t = t_i'$, for $i = \overline{1, N_T}$, obtained from the BEM solution of the direct problem, as described in Section 3, by using the estimated values of the unknown parameters $(\mathbf{C}, \mathbf{k})$.

As will be seen later in Section 5 when the numerical method will be experimented for several values of N_T in the Example 5.1, in expression (15) the number of measurements should, in general, be equal or exceed the number of unknowns and this fact is consistent with the numerical experiments from [24] for the estimation of spatially varying thermal properties.

Additional physical constraints are imposed, namely,

$$C(T) \geq 0, \quad k(T) \geq 0. \quad (16)$$

Temperature dependent uniqueness conditions applicable to the problem of estimating $C(T)$ and $k(T)$ are very difficult (see [9–11]) and in order to be able to obtain a unique solution, $C(T)$ and $k(T)$ have to be fixed at some points. This restriction should ensure uniqueness of the estimated thermal property parameters and this will be discussed further in Section 5.

Finally, the stability of the solution is ensured since the number of independent parameters which are to be estimated, i.e., the dimension of the space $\mathbb{F}$, is, in general, small and no further regularization term is needed in the expression for the functional (15); see also [25]. The minimization of the nonlinear least-squares functional (15), subject to the positivity constraints (16) and to the additional fixing conditions, is solved using the NAG routine E04UCF (see [26]) which minimizes an arbitrary smooth function subject to certain constraints which may include simple bounds on variables and linear or nonlinear constraints. At this stage it should be noted that other methods, such as the Levenberg–Marquad method of minimization and the iterated conjugate gradient method (see [7, 27]) would have been more effective and cheaper in computational time, since they are to be supplied by the user. However, in this study the minimization with constraints implemented in the NAG routine has been preferred as it was easy to use, is robust and reasonably efficient since it is based on a sequential quadratic programming method developed in [28].

5. NUMERICAL RESULTS AND DISCUSSION

The numerical inversion method for the identification of the thermal conductivity and the heat capacity, as described in the Sections 3 and 4, has been applied to various test examples in which the space $\mathbb{F}$ is the set of constant, linear or quadratic functions. Also the identification procedure provides simultaneously the temperature inside the solution domain and the boundary heat flux.

In all the examples performed in this section we will interpret the results obtained by considering the material to be an alloy of steel with a reference thermal diffusivity $a_r = k_r/C_r = 10^{-5}$ m^2/s, of length $l = 0.06$ m, and subject to a heat conducting experiment over a period of time $t_f = 360$ s. The boundary temperature is assumed to be known from

$$\Delta t^* = t^*_{i+1} - t^*_i = t_f(t_{i+1} - t_i) = t_f\,\Delta t \quad (\mathrm{s}) \tag{17a}$$

whilst temperature measurements at $x^* = d^* = dl = 0.03$ m are recorded at a sampling rate of

$$\Delta t'^* = t'^*_{i+1} - t'^*_i = t_f(t'_{i+1} - t'_i) = t_f/N_T \quad (\mathrm{s}). \tag{17b}$$

Also, in all the test examples presented in this section the value of d at which the temperature sensor is located was taken to be equal to 0.5, although alternative choices of $d \in (0, 1)$ do not significantly affect the accuracy of the results. The distance d is important in the sensitivity analysis of the IHCP (see [29]), but not in the IDHCP. Further, for the IDHCP the Fourier number $\Lambda = d(a_r\,\Delta t^*)^{-1/2}$ does not seem to be meaningful as the distance d should be related to an active boundary which does not appear in the formulation of the IDHCP considered in this study. That is to say that the IHCP is a boundary inverse problem, whilst the IDHCP is a coefficient identification (inverse) problem.

For exact measured data $T^{(m)}(t)$, in order to test the accuracy and convergence of the numerical method, the examples are analysed for various numbers of time measurements, $N_T \in \{1, 2, 4, 5, 10, 20\}$, and/or various time steps, $\Delta t \in \{0.025, 0.05, 0.1\}$. For the alloy of steel material, this corresponds to the boundary temperature being known from $\Delta t^* \in \{9, 18, 36\}$ s and temperature measurements being recorded at various sampling rates of $\Delta t'^* \in \{360, 180, 90, 72, 36, 18\}$ s. It should be noted that all these physical and technical quantities are practically realistic and they are of the same order as those considered in the simulated tests performed in [12].

Also, in order to test the stability of the numerical method that one has employed, various amounts of noise, $p\% \in \{0, 2, 4, 6, 8\}$, are included in the measured data $T^{(m)}(t)$ at $x = d$.

EXAMPLE 5.1. Initially, we consider a simple test example in which

$$C(T) = 1, \quad k(T) = k_1 + k_2 T, \tag{18a}$$

$$f_0(t) = \varepsilon t, \quad f_1(t) = 1 + \varepsilon t, \quad T_0(x) = x,$$

$$T^{(m)}(t) = 0.5 + \varepsilon t, \tag{18b}$$

where $\varepsilon > 0$ is an arbitrary preassigned constant and k_1 and k_2 are constant coefficients to be determined.

At this stage, we note that although the linear dependence of $k(T)$ with T given by expression (18a) may appear very simple, many materials possess such a linear variation of their thermal conductivity with the temperature over a large temperature range (see, for example, [14]).

With the data (18) it is required then to numerically solve the problem (1), which possesses the analytical solution

$$T(x, t) = x + \varepsilon t, \quad C(T) = 1, \quad k(T) = k_1 + \varepsilon T. \tag{19}$$

From expression (19) it can be seen that in order to obtain a unique solution, $k(T)$ should be fixed at one point and we have set, for convenience,

$$k(0) = k_1 = 1. \tag{20}$$

TABLE I

The Numerical Results for k_2 and the Objective Values Obtained Using a Time Step $\Delta t = 0.05$ for Various Values of $\varepsilon \in \{0.5, 1, 2\}$ and $N_T \in \{1, 2, 4, 5, 10, 20\}$ for Example 5.1

$\Delta t = 0.05$	$N_T = 1$	$N_T = 2$	$N_T = 4$	$N_T = 5$	$N_T = 10$	$N_T = 20$	Analytical ε
k_2	0.50259	0.50276	0.50266	0.50259	0.50239	0.50221	0.5
	1.02571	1.02216	1.02093	1.02059	1.01971	1.01913	1
	2.53260	2.27088	2.20619	2.19715	2.18288	2.17685	2
$S(\mathbf{C}, \mathbf{k})$	0.1E-25	0.5E-10	0.18E-8	0.58E-8	0.77E-7	0.53E-6	0
	0.1E-22	0.47E-7	0.89E-7	0.12E-6	0.47E-6	0.24E-5	0
	0.1E-25	0.13E-4	0.28E-4	0.34E-4	0.63E-4	0.12E-3	0

In developing the BEM, both in the direct and inverse analysis, we need the generic form of the Kirchhoff transformation $\Psi(T)$, given by expression (3), which for the particular form of the thermal conductivity given by expression (18a), results in

$$\Psi(T) = k_1 T + k_2 T^2/2. \tag{21}$$

Also, in order to calculate the original temperature distribution T, using expression (13), Eq. (21) is inverted to give

$$\Psi^{-1}(\psi) = ((k_1^2 + 2k_2\psi)^{1/2} - k_1)/k_2. \tag{22}$$

In inverting Eq. (21) only the positive root was selected since the negative root leads to a value of T which corresponds to a negative thermal conductivity, which has no physical meaning. If an analytical inversion of Eq. (21) is not possible then a numerical technique has to be employed.

Table I shows the numerical results obtained for k_2 using a constant time step $\Delta t = 0.05$ for various values of $\varepsilon \in \{0.5, 1, 2\}$ and various numbers of time measurements $N_T \in \{1, 2, 4, 5, 10, 20\}$. Also, in all the tables shown in this section the optimal values of the objective function, $S(\mathbf{C}, \mathbf{k})$, given by expression (15), which is minimized and the analytical values are included. From Table I it can be seen that as the number of time measurements, N_T, increases the agreement between the analytical and numerical values of k_2 improves as more constraint information is imposed on the solution of the inverse problem. This improvement is much enhanced for the situation when $\varepsilon = 2$, where the relative error decreases from about 25% for $N_T = 1$ to about 9% when $N_T = 20$. As the value of ε decreases, i.e., the thermal diffusivity dependence on the temperature becomes weaker, the relative error and the objective value, $S(\mathbf{C}, \mathbf{k})$, for a fixed value of N_T, decrease. The number of time measurements should exceed, in general, the number of unknowns and, since in all the examples tested in this section the number of parameters to be estimated is less than four, a typical value of $N_T = 10$ was adopted throughout as this was found to be sufficiently large to ensure the accuracy of the results. A larger value of N_T will not significantly improve the results and, in addition, there might be practical limitations in the period of the time sampling measurements, $\Delta t'^*$, that can be taken by a sensor installed inside a heated conducting body. Finally, although for $\varepsilon = 2$ the relative error for $N_T = 10$ is still large, about 9%, better agreement with the analytical solution may be achieved by decreasing the time step, Δt, i.e., by decreasing the sampling rate Δt^* at which the boundary temperature is assumed to be known.

Table II shows the numerically obtained results for k_2 for various values of $\varepsilon \in \{0.5, 1, 2\}$ and for various time steps $\Delta t \in \{0.025, 0.05, 0.1\}$. It can be seen that as the time step decreases in size, the numerical results converge to the analytical value of k_2 and also the objective values tend to zero. Also, as the value of ε decreases, then the rate of convergence to the analytical solution improves. This is to be expected since as ε decreases the problem becomes less nonlinear. For $\varepsilon = 2$ the enhanced decrease in the relative error is from 44% for $\Delta t = 0.1$, to 9% for $\Delta t = 0.05$, and to 2% for $\Delta t = 0.025$. From this discussion it can be concluded that if the time step is sufficiently decreased, the numerical method based on the BEM approach, may

TABLE II

The Numerically Obtained Results for k_2 and the Objective Values for Various Values of $\varepsilon \in \{0.5, 1, 2\}$ and Time Steps $\Delta t \in \{0.025, 0.05, 0.1\}$ for Example 5.1

	Time step Δt			
$N_T = 10$	0.1	0.05	0.025	Analytical ε
k_2	0.51413	0.50239	0.50082	0.5
	1.09421	1.01971	1.00584	1
	2.88493	2.18288	2.04357	2
$S(\mathbf{C}, \mathbf{k})$	0.13E-5	0.77E-7	0.78E-8	0
	0.21E-4	0.47E-6	0.15E-7	0
	0.17E-2	0.63E-4	0.73E-4	0

TABLE IIIa

The Numerical Results for the Temperature at Some Interior Domain Points Obtained Using the Time Steps $\Delta t \in \{0.025, 0.05, 0.1\}$ for Example 5.1 when $\varepsilon = 0.5$

		Time step Δt			
x	t	0.1	0.05	0.025	Analytical
0.2125	0.2	0.31074	0.31283	0.31364	0.3125
0.4125	0.2	0.51196	0.51284	0.51299	0.5125
0.6125	0.2	0.71021	0.71156	0.71179	0.7125
0.8125	0.2	0.90643	0.90983	0.91105	0.9125
0.2125	0.4	0.41044	0.41264	0.41351	0.4125
0.4125	0.4	0.61164	0.61272	0.61293	0.6125
0.6125	0.4	0.80998	0.81153	0.81182	0.8125
0.8125	0.4	1.00630	1.00983	1.01110	1.0125
0.2125	0.6	0.51028	0.51252	0.51340	0.5125
0.4125	0.6	0.71155	0.71268	0.71290	0.7125
0.6125	0.6	0.90996	0.91156	0.91186	0.9125
0.8125	0.6	1.10631	1.10986	1.11115	1.1125
0.2125	0.8	0.61014	0.61241	0.61331	0.6125
0.4125	0.8	0.81147	0.81266	0.81287	0.8125
0.6125	0.8	1.00995	1.01159	1.01190	1.0125
0.8125	0.8	1.20631	1.20989	1.21119	1.2125

TABLE IIIb

The Numerical Results for the Temperature at Some Interior Domain Points Obtained Using the Time Steps $\Delta t \in \{0.025, 0.05, 0.1\}$ for Example 5.1 when $\varepsilon = 1$

		Time step Δt			
x	t	0.1	0.05	0.025	Analytical
0.2125	0.2	0.40871	0.41332	0.41525	0.4125
0.4125	0.2	0.60919	0.61272	0.61359	0.6125
0.6125	0.2	0.80458	0.80956	0.81077	0.8125
0.8125	0.2	0.99702	1.00573	1.00897	1.0125
0.2125	0.4	0.60759	0.61242	0.61444	0.6125
0.4125	0.4	0.80848	0.81244	0.81335	0.8125
0.6125	0.4	1.00439	1.00978	1.01108	1.0125
0.8125	0.4	1.19705	1.20598	1.20932	1.2125
0.2125	0.6	0.80673	0.81181	0.81386	0.8125
0.4125	0.6	1.00805	1.01228	1.01320	1.0125
0.6125	0.6	1.20435	1.20998	1.21132	1.2125
0.8125	0.6	1.39716	1.40617	1.40957	1.4125
0.2125	0.8	1.00596	1.01132	1.01342	1.0125
0.4125	0.8	1.20757	1.21213	1.21309	1.2125
0.6125	0.8	1.40419	1.41009	1.41149	1.4125
0.8125	0.8	1.59716	1.60629	1.60974	1.6125

deal with stronger nonlinearities when the thermal diffusivity varies linearly with the temperature. This is probably because for this test example the approximation of $a(T)$, with its mean average value given by expression (8), improves as the time step decreases. At the final iteration at which the thermal properties have been determined, to within some specified accuracy, the time marching BEM provides also the temperature field inside the solution domain.

Tables IIIa, IIIb, and IIIc show the numerical results for the temperature at some interior domain points obtained using the BEM time marching technique with various time steps $\Delta t \in \{0.025, 0.05, 0.1\}$ in comparison with the analytical solutions for $\varepsilon = 0.5, 1$, and 2, and $k_1 = 0.50082, 1.00584$, and 2.04357 (see Table II), respectively. It can be seen that the agreement between the numerical results and the analytical solution is very good and this illustrates that the BEM solution of the direct problem is stable with respect to thermal conductivity data. The stability is suggested by the fact that although the values of k_2 are in relative error by about 0.1%, 0.5%, and 2% from their exact values for $\varepsilon = 0.5$, 1, and 2, respectively, see Table II, these errors do not amplify but are damped when calculating the temperature distribution inside the solution domain. In all Tables III it can be seen that the numerical results for the temperature at all the selected points increase as the time step decreases. This monotonic increasing sequence of numerically obtained temperature results appears to converge to the corresponding analytical values for points situated, in general, away from the boundary $x = 0$. At other points near the boundary $x = 0$ this convergence does not appear straightforward and this is probably because in the nonlinear formulation of the BEM domain integrals due to the gradients of the thermal diffusivity, which may not necessarily decay to zero at all the domain points as

TABLE IIIc

The Numerical Results for the Temperature at Some Interior Domain Points Obtained Using the Time Steps $\Delta t \in \{0.025, 0.05, 0.1\}$ for Example 5.1 when $\varepsilon = 2$

		Time step Δt			
x	t	0.1	0.05	0.025	Analytical
0.2125	0.2	0.59900	0.61161	0.61623	0.6125
0.4125	0.2	0.79621	0.81047	0.81429	0.8125
0.6125	0.2	0.98663	1.00456	1.00979	1.0125
0.8125	0.2	1.17321	1.19662	1.20554	1.2125
0.2125	0.4	0.99465	1.00891	1.01365	1.0125
0.4125	0.4	1.19428	1.20974	1.21363	1.2125
0.6125	0.4	1.38653	1.40527	1.41063	1.4125
0.8125	0.4	1.57369	1.59747	1.60641	1.6125
0.2125	0.6	1.39033	1.40698	1.41222	1.4125
0.4125	0.6	1.59123	1.60866	1.61310	1.6125
0.6125	0.6	1.78485	1.80503	1.81085	1.8125
0.8125	0.6	1.97301	1.99759	2.00671	2.0125
0.2125	0.8	1.78645	1.80539	1.81128	1.8125
0.4125	0.8	1.98802	2.00746	2.01263	2.0125
0.6125	0.8	2.18265	2.20440	2.21082	2.2125
0.8125	0.8	2.37182	2.39737	2.40678	2.4125

TABLE IV

The Numerical Results for k_1, k_2, and k_3 and the Objective Values for the Time Steps $\Delta t \in \{0.025, 0.05, 0.1\}$ for Example 5.2

	Time step Δt			
$N_T = 10$	0.1	0.05	0.025	Analytical
k_1	5.73E-3	4.09E-3	3.79E-3	0
k_2	0.49238	0.49549	0.49612	0.5
k_3	0.06436	0.06290	0.06257	0.0625
$S(\mathbf{C}, \mathbf{k})$	0.45E-7	0.13E-8	0.77E-9	0

the time step tends to zero, have been neglected. However, the BEM approach is more than reasonable since, from all the values of the nonlinearity coefficient ε and all the time steps considered in Tables III, the numerical estimation of the interior temperature agrees to within 1–2% with the analytical solution.

EXAMPLE 5.2. In the second test example we consider a higher (quadratic) temperature dependence for the thermal diffusivity, namely, we take

$$C(T) = 1, \quad k(T) = k_1 + k_2 T + k_3 T^2 \tag{23a}$$

$$f_0(t) = (t/2)^{1/2}, \quad f_1(t) = (4 + t/2)^{1/2}, \quad T_0(x) = 2x^{1/2},$$
$$T^{(m)}(t) = (2 + t/2)^{1/2}, \tag{23b}$$

where k_1, k_2, and k_3 are constant coefficients to be determined.

With the data (23), it is required to numerically solve the problem (1) which possesses the analytical solution

$$\begin{aligned} T(x,t) &= (4x + t/2)^{1/2}, \quad C(T) = 1, \\ k(T) &= k_2 T + 0.0625 T^2. \end{aligned} \tag{24}$$

From expression (24) it can be seen that in order to obtain a unique solution, $k(T)$ should be fixed at one point, and we have set, for convenience,

$$k(1) = k_1 + k_2 + k_3 = 0.5625. \tag{25}$$

For the quadratic representation (23a), the Kirchhoff transformation is given by

$$\Psi(T) = k_1 T + k_2 T^2/2 + k_3 T^3/3. \tag{26}$$

The inversion of Eq. (26) is based on Cardano's formulae (see, for example, [30]) and the function $\Psi^{-1}(\psi)$ is then defined as the unique root which produces positive values for the thermal conductivity.

Table IV shows the numerical results for k_1, k_2, and k_3 for various time steps, $\Delta t \in \{0.025, 0.05, 0.1\}$. It can be seen that the numerical values of k_1, k_2, and k_3 converge towards their corresponding analytical values as the time step decreases. Also, it is observed that the objective values appear to converge towards zero.

Figures 1a and 1b show the numerically obtained results for the heat flux at the boundaries $x = 0$ and $x = 1$, respectively, in comparison with the corresponding analytical solutions for the time steps $\Delta t \in \{0.025, 0.05, 0.1\}$. In Fig. 1a the heat flux at $x = 0$ is infinite as t tends to zero and the BEM predicts this behaviour as the time step decreases. The numerical solution, represented by symbols calculated at the nodes of each time element, appears to lie on the analytical curve, as shown in Fig. 1a, but because of the large scale used for the heat flux, $q(0, t)$, we show in Fig. 1b the boundary heat flux $q(1, t)$. It can be observed that there is an approximately constant relative error of about 1% between the numerical and analytical solutions. This error does not diminish as the time step decreases in size and is not caused by errors in the calculated values of k_1, k_2, and k_3 as the direct numerical solution with exact values for these coefficients, represented by the dotted line, shows. This inconsistency is probably because in this test example the thermal diffusivity depends more than weakly on the temperature and therefore the domain integrals involving the gradients of $a(T)$ are significant. Although the BEM formulation itself is approximate in the nonlinear transient case with thermal diffusivity temperature dependence (see [31]), this approximation is still reasonable as it estimates, to within about 1%, the analytical solution (see also Example 5.1). In addition, in the well-posed direct problem of heat conduction the small errors in the boundary value data will be damped when calculating the temperature inside the solution domain due to the diffusive nature of the parabolic heat conduction equation.

EXAMPLE 5.3. In the third test example we consider the case in which both the heat capacity and the thermal conductivity are temperature dependent, namely,

$$C(T) = C_1 + C_2 T, \quad K(T) = k_1 + k_2 T \tag{27a}$$

$$f_0(t) = ((1 + 8t)^{1/2} - 1)/2, \quad f_1(t) = ((5 + 8t)^{1/2} - 1)/2,$$
$$T_0(x) = ((1 + 4x^2)^{1/2} - 1)/2 \tag{27b}$$

$$T^{(m)}(t) = ((2 + 8t)^{1/2} - 1)/2 + \mu(t), \tag{27c}$$

where C_1, C_2 and k_1, k_2 are constant coefficients to be determined and $\mu(t)$ is a random function which in the computation is implemented as a discrete vector of random variables $\mu(t_i') = \mu_i$ for $i = \overline{1, N_T}$, generated by the NAG routine G05DDF (see [32]) with mean zero and standard

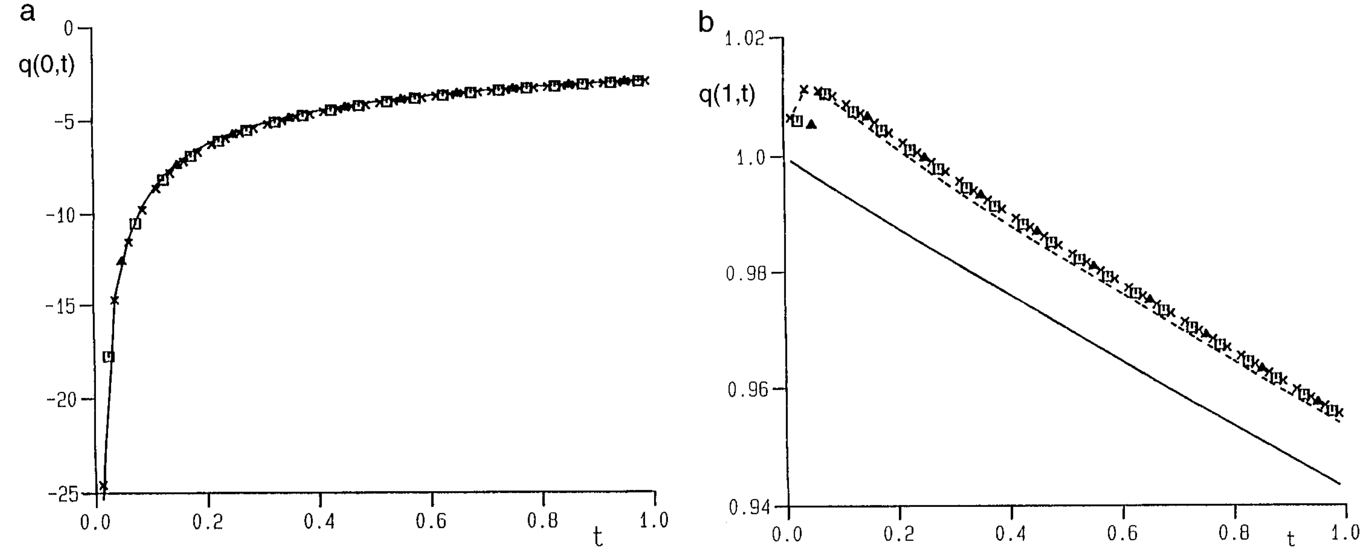

FIG. 1. The results for the boundary heat flux, namely, (a) $q(0, t)$ at $x = 0$; (b) $q(1, t)$ at $x = 1$, for Example 5.2, obtained using: (△△△) the numerical solution with $\Delta t = 0.1$; (□□□) the numerical solution with $\Delta t = 0.05$; (×××) the numerical solution with $\Delta t = 0.025$; (---) the direct BEM solution with exact values of the thermal conductivity and $\Delta t = 0.025$; (———) the analytical solution.

deviation σ_i taken to be some percentage $p\%$ from the absolute temperature at $x = d$ at the time t_i', namely,

$$\sigma_i = \frac{p}{100}|T(d, t_i')|, \quad i = \overline{1, N_T}. \tag{28}$$

With the data (27) it is required to numerically solve the problem (1) which possesses the analytical solution

$$\begin{aligned} T(x,t) &= ((1 + 4(x^2 + 2t))^{1/2} - 1)/2, \\ C(T) &= C_1 + 2T, \quad k(T) = k_1 + 2T. \end{aligned} \tag{29}$$

From the expressions (29) it can be seen that in order to obtain a unique solution then $C(T)$ and $k(T)$ should both be fixed at one point which for the purpose of this example is set to be

$$C(0) = C_1 = k(0) = k_1 = 1. \tag{30}$$

This quasi-linear test example was chosen in order to investigate the case of temperature dependent heat capacity and thermal conductivity but with constant thermal diffusivity. In this case, in the direct problem the Kirchhoff transformation (3) will reduce the problem to a linear heat conduction Eq. (5a) for which the BEM is applicable in its exact formulation. However, in the inverse analysis the problem still remains nonlinear during the iterative procedure and it is the purpose of this example to investigate the retrieval of the linear case solution. Also, the effect of various amounts of noise p is investigated in order to test the stability of the numerical inversion method that one has employed.

Table V shows the numerical results for C_2 and k_2 for the time steps $\Delta t \in \{0.025, 0.05, 0.1\}$ and no noise, i.e., $p = 0$, included in the data (27c). Although the results obtained with the large time step $\Delta t = 0.1$ have about an 8% relative error with respect to the analytical values, as the time step decreases to $\Delta t = 0.025$ the relative error decreases to about 1%. The convergence is monotonic and the same conclusion may be drawn for the objective values. Also, the approximation of the thermal conductivity coefficient k_2 is slightly better than the approximation for the heat capacity coefficient C_2. Further, although not illustrated, the same monotonic increasing convergence of the numerical results for the temperature at some interior domain points obtained using the BEM marching technique for the time steps $\Delta t \in \{0.025, 0.05, 0.1\}$ towards the analytical solution has been achieved. Furthermore, as the numer-

TABLE V

The Numerical Results for C_2 k_2 and the Objective Values for the Time Steps $\Delta t \in \{0.025, 0.05, 0.1\}$ for Example 5.3

	Time step Δt			Analytical
$N_T = 10$	0.1	0.05	0.025	ε
C_2	1.84001	1.95069	1.98804	2
k_2	1.87890	1.95899	1.99127	2
$S(\mathbf{C}, \mathbf{k})$	0.23E-5	0.11E-6	0.79E-8	0

TABLE VI

The Numerical Results for C_2, k_2, the Objective Values $S(\mathbf{C}, \mathbf{k})$, the Time Consuming on a SUN Workstation, and the Number of Iterations Obtained Using the Time Step $\Delta t = 0.025$ and the Initial Guesses $C_2 = 0.5$ and $k_2 = 1.5$, for Example 5.3 when Various Amounts of Noise $p \in \{0, 2, 4, 6, 8\}$ Are Included in the Measured Data $T^{(m)}(t)$ Given by Expression (27c)

$N_T = 10$ $\Delta t = 0.025$	C_2	k_2	$S(\mathbf{C}, \mathbf{k})$	Time consuming (in seconds)	Number of iterations
Analytical	2	2	0	0	0
$p = 0$	1.98804	1.99127	0.79E-8	1033	18
$p = 2$	2.09673	1.96644	0.16E-2	1131	15
$p = 4$	2.17685	1.91947	0.65E-2	1724	15
$p = 6$	2.22552	1.85020	0.14E-1	974	14
$p = 8$	2.24009	1.75870	0.26E-1	944	15

ical values of C_2 and k_2 converge to the same value it follows that the thermal diffusivity becomes constant and in this case the inconsistency observed in the previous example is not present since the BEM is exactly formulated in the linear or quasi-linear cases. Finally, for Example 5.3 when various amounts of noise $p \in \{0, 2, 4, 6, 8\}$ are included in the measured data (27c), Table VI shows the numerical results for C_2, k_2, and $S(\mathbf{C}, \mathbf{k})$, obtained using the time step $\Delta t = 0.025$. Also included in this table are the values of the computational time taken, in seconds, on a SUN workstation at the University of Leeds and the number of iterations required for convergence by the NAG routine E04UCF when the initial guesses for C_2 and k_2 were 0.5 and 1.5, respectively. From Table VI it can be seen that the numerical estimation of the thermal properties is stable with respect to the noise in the measured data $T^{(m)}(t)$ and also that this estimation becomes better in comparison with the analytical values as the data $T^{(m)}(t)$ is known more precisely, i.e., as p decreases.

For all the examples presented in this section representing various heat-conducting materials formed from alloys of steel, it was found that if the boundary temperatures are known with a period of sampling of $\Delta t^* \leq 9$ s and if the temperature measurements taken with a sensor installed at an arbitrary position within the material are available, within tolerancies of $p\% \leq 8\%$, with a period of sampling of $\Delta t'^* \cong 36$ s, then the numerical inversion method produced good and stable estimates for the unknown thermal properties of the material and also for the interior temperature solution and the boundary heat fluxes. This concludes the fact that the numerical inversion method produces good performance in estimating the thermal properties of heated materials, whilst allowing large periods of practical sampling measurements and reasonably large tolerancy errors permitted to the experimentalist.

6. CONCLUSIONS

The present study has investigated using the BEM, the nonlinear inverse problem of the simultaneous identification of the thermal conductivity, the heat capacity, and the temperature solution from additional time temperature measurements taken at an arbitrary location within a heated conducting body. In comparison with the full domain discretisation methods, the BEM is well-suited and advantageous for discretising this class of inverse problems since no solution domain discretisation, no interpolation on the grid cells when calculating the temperature measurements at arbitrary points within, or on the boundary of the heated body, no further finite differencing for obtaining the boundary heat flux and no fundamental distinction in the principle of implementation of the method when changing the types of boundary conditions, are required. Based on the Kirchhoff transformation and assuming that the thermal diffusivity is weakly temperature dependent, a time marching BEM has been developed using an iterative procedure. In general, the inverse identification problem is ill-posed since it has no unique solution and in order to render a unique solution then additional constraints have to be imposed. Additional interior temperature measurements are known and also the thermal properties are assumed to belong to a finite-dimensional space, such as the space of constant, linear, or quadratic polynomials. The parameter estimation thermal properties problem has been solved by minimizing the nonlinear least-squares functional, subject to certain constraints which include the physical quantities being positive and fixing conditions for the unknowns. For various test examples representing heat conducting materials formed from alloys of steel it has been found that the numerical method always gives an accurate, convergent, and stable solution for the thermal properties' coefficients with increasing accuracy, as the time step decreases, as the number of time measurements increase, and also as the measured data is known more precisely. In addition, good estimates for the thermal properties may be obtained, provided that the time step is sufficiently small, even for strong linear dependences on temperature of the thermal diffusivity. Also, the numerical results for the temperature inside the solution domain show good estimates of the corresponding analytical solution. All these conclusions are even more encouraging as the numerical inversion method produces good performances in estimating the thermal properties of heated materials and the temperature solution, whilst allowing large periods of practical sampling measurements and reasonably large tolerancy errors permitted to the experimentalist. Furthermore, the BEM can be extended to deal with higher dimensions and nonlinear boundary conditions.

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