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An inverse problem in simultaneously measuring temperature-dependent thermal conductivity and heat capacity

CHENG-HUNG HUANG and JAN-YUAN YAN

Department of Naval Architecture and Marine Engineering, National Cheng Kung University, Tainan, Taiwan, Republic of China

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Abstract—An inverse analysis utilizing the conjugate gradient method of minimization and the adjoint equation is used for simultaneously estimating the temperature-dependent thermal conductivity and heat capacity per unit volume of a material. No prior information is used for the functional forms of the unknown thermal conductivity and heat capacity in the present study, thus, it is classified as the function estimation by inverse calculation. The accuracy of the inverse analysis is examined by using simulated exact and inexact measurements obtained within the medium. Results show that the CPU time used on a VAX-9420 computer is within 1.4–4.46 s for all the test cases considered here. Moreover, excellent estimations on the thermal properties can be obtained when a good initial guess of either thermal conductivity or heat capacity is given before the inverse calculations.

1. INTRODUCTION

Thermal heat transport in materials is governed by thermophysical properties such as the thermal conductivity and heat capacity. The magnitude of these properties has a significant influence on the analysis of temperature distribution and heat flow rate when the material is heated and also on the analysis of thermal instability problems. Many theoretical and experimental methods for measuring the thermophysical properties have been developed in the literature, they include, among others, the steady-state method [1], the probe method [2, 3], the periodic heating method [4, 5], the least-squares method [6, 7] and the pulse heating method [8, 9]. However, all the above references belong to either steady-state or parameter estimations. The transient function estimation for simultaneously measuring temperature-dependent thermal conductivity and heat capacity per unit volume, using the conjugate gradient method in an inverse heat conduction problem, has never been examined in the open literature.

The present work addresses the development of an efficient method (i.e. the conjugate gradient method) of analysis for measuring the temperature-dependent thermal conductivity and heat capacity of a material. Multiple spatial and temporal temperature measurements are found to be needed in transient heat conduction experiments. Besides, no *a priori* information on the functional forms of the unknown quantities is necessary in inverse calculations.

Alifanov [10] was among the early users of the conjugate gradient method. More recently, the method has been used for solving inverse problems of determining: the wall heat flux in laminar flow through a parallel plate duct [11]; interface conductance between mold and casting during solidification [12]; interface conductance between periodically contacting surface [13]; wall heat fluxes of a hollow cylinder [14]; and heat fluxes inside the cylinder of an internal combustion engine [15].

The conjugate gradient method is derived from perturbation principles [10] and transforms the inverse problem to the solution of three problems, namely, the direct problem, the sensitivity problem and the adjoint problem, which will be discussed in the following sections.

2. DIRECT PROBLEM

To illustrate the methodology for developing expressions for use in simultaneously determining unknown temperature-dependent thermal conductivity, $k(T)$ and heat capacity per unit volume, $C(T)$, in a material, we consider the following transient inverse heat conduction problem. A slab of thickness $\bar{L}$ is initially at temperature $\bar{T}(\bar{x}, 0) = \bar{T}_0$. For time $\bar{t} > 0$, the boundary surface at $\bar{x} = 0$ is subjected to a prescribed constant heat flux $\bar{q}_1$, while at boundary $\bar{x} = \bar{L}$, a constant heat flux $\bar{q}_2$ is removed from the slab by cooling. Figure 1(a) shows the geometry and the coordinates for the one-dimensional physical problem considered here.

If the following dimensionless quantities are defined

$$x = \frac{\bar{x}}{\bar{L}} \quad T = \frac{\bar{T}}{\bar{T}_r} \quad T_0 = \frac{\bar{T}_0}{\bar{T}_r} \quad k = \frac{\bar{k}}{\bar{k}_r}$$

$$q = \frac{\bar{L}}{\bar{k}_r \bar{T}_r}\bar{q} \quad t = \frac{\bar{k}_r}{\bar{\rho}\bar{C}_r \bar{L}^2}\bar{t} \quad C = \frac{\bar{C}}{\bar{C}_r}$$

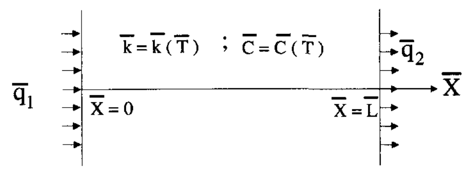
NOMENCLATURE

$C(T)$ or $C(x,t)$ unknown heat capacity per unit volume
J functional defined by equation (2)
J' gradient of functional defined by equations (12c) and (12d)
$k(T)$ or $k(x,t)$ unknown thermal conductivity
P direction of descent defined by equations (3c) and (3d)
$T(x,t)$ estimated dimensionless temperature
$\Delta T(x,t)$ sensitivity function defined by equations (4) and (5)
$Y(x,t)$ measured temperature.

Greek symbols
β search step size
γ conjugate coefficient
$\delta(\cdot)$ Dirac delta function
ε convergence criteria
$\lambda(x,t)$ Lagrange multiplier defined by equation (11)
ω random number.

Superscript
$\hat{}$ estimated values
$\bar{}$ dimensional parameters
n iteration index.

Subscript
r reference parameters.



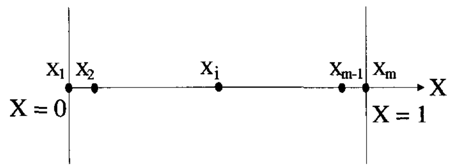


Fig. 1. (a) Physical problem; (b) thermocouple arrangement for m points measurements.

the dimensionless formulation of this transient heat conduction problem can be expressed as:

$$\frac{\partial}{\partial x}\left(k(T)\frac{\partial T(x,t)}{\partial x}\right) = C(T)\frac{\partial T(x,t)}{\partial t} \quad \text{in } 0 < x < 1 \tag{1a}$$

$$-k(T)\frac{\partial T(x,t)}{\partial x} = q_1 \quad \text{at } x = 0 \tag{1b}$$

$$-k(T)\frac{\partial T(x,t)}{\partial x} = q_2 \quad \text{at } x = 1 \tag{1c}$$

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

where the superscript '$^-$' and subscript 'r' denote the dimensional and referenced quantities, respectively. We assume $\bar{T}_0 = \bar{T}_r$, i.e. $T_0 = 1$ in the direct problem (1). The above quantities are assumed known while $k(T)$ and $C(T)$ are the unknown temperature-dependent thermal properties that are to be determined.

When generating simulated temperature measurements $T(x,t)$, i.e. given $k(T)$ and $C(T)$ to calculate temperature $T(x,t)$, the direct problem (1) is nonlinear since thermal properties are functions of temperature, therefore an iterative technique is needed in solving the problem with the finite-difference method. At this stage, $k(T)$ and $C(T)$ cannot be replaced by $k(x,t)$ and $C(x,t)$, since $k(T)$ and $C(T)$ are unknown before the direct problem calculations. However, when the temperatures $T(x,t)$ are converged by an iterative technique under some specified initial and boundary conditions, the values of k and C at any time and position, (x,t), should be fixed because temperatures $T(x,t)$ are known and fixed at any (x,t).

Now, in the inverse calculations considered here, the measurement temperatures $T(x,t)$ are assumed known either from numerical simulations or from real experiments. Once $T(x,t)$ are obtained, there exist some unknown but fixed exact thermal properties that their values (a number), $k(x,t)$ and $C(x,t)$, at any specific time and position, (x,t), must satisfy in the Fourier equation to give this known temperature distribution $T(x,t)$.

Therefore, in the inverse problem of function estimations, one can first guess the values of $\hat{k}(x,t)$ and $\hat{C}(x,t)$, then by using the minimization procedure described in the following sections one can minimize the cost function J and finally find the exact $k(x,t)$ and $C(x,t)$.

If the values of $k(x,t)$ and $C(x,t)$ can be predicted correctly before the direct problem calculation, it becomes a linear problem and the iterative procedure is not needed in computing the direct problem.

The direct problem considered here is concerned with the determination of the medium temperature when the thermal properties and the boundary conditions at $x = 0$ and $x = 1$ are known.

3. INVERSE PROBLEM

For the inverse problem, the thermal properties $k(x, t)$ and $C(x, t)$ are regarded as being unknown, but everything else in equation (1) is known. In addition, temperature readings taken at some appropriate locations are considered available.

Referring to Fig. 1(b), we assumed that m sensors are used to record the temperature information to identify $k(x, t)$ and $C(x, t)$ in the inverse calculations. Let the temperature readings taken within these sensors over the time period t_f be denoted by $Y_i(x_i, t) \equiv Y_i(t)$, $i = 1$ to m, where $i = 1$ and m always correspond to $x = 0$ and 1 (i.e. boundary measurements) respectively. Then the inverse problem can be stated as follows: by utilizing the above-mentioned measured temperature data, $Y_i(t)$, estimate the unknown thermal properties, $k(x, t)$ and $C(x, t)$, over t_f.

Since all the measured temperatures are used to compute the entire unknown functions for one period of time variation and no *a priori* information is available on the functional forms of $k(x, t)$ and $C(x, t)$, the method used here may be classified as the function estimation in the whole-domain [16] for the determination of the nonlinear thermal properties, $k(T)$ and $C(T)$.

The solution of the present inverse problem is to be obtained in such a way that the following functional is minimized:

$$J[k(T), C(T)] \equiv J[k(x, t), C(x, t)]$$

$$= \int_{t=0}^{t_f} \sum_{i=1}^{m} [T_i(x_i, t) - Y_i(x_i, t)]^2 \, dt \quad (2)$$

here, T_i are the estimated temperatures in the slab at the measured locations $x = x_i$. These quantities are determined from the solution of the direct problem given previously using an estimated $\hat{k}(x, t)$ and $\hat{C}(x, t)$ for the exact $k(x, t)$ and $C(x, t)$ respectively. Here the superscript '^' denotes the estimated quantities.

4. CONJUGATE GRADIENT METHOD FOR MINIMIZATION

The following iterative process based on the conjugate gradient method [10] is now used for the estimations of $k(x, t)$ and $C(x, t)$ by minimizing the above functional $J[k(x, t), C(x, t)]$

$$\hat{k}^{n+1}(x, t) = \hat{k}^n(x, t) - \beta_k^n P_k^n(x, t) \quad \text{for } n = 0, 1, 2, \ldots \quad (3a)$$

$$\hat{C}^{n+1}(x, t) = \hat{C}^n(x, t) - \beta_C^n P_C^n(x, t) \quad \text{for } n = 0, 1, 2, \ldots \quad (3b)$$

where β_k^n and β_C^n are two search step sizes for k and C in going from iteration n to iteration $n+1$, and P_k^n and P_C^n are the directions of descent (i.e. search direction) for k and C given by

$$P_k^n(x, t) = J_k'^n(x, t) + \gamma_k^n P_k^{n-1}(x, t) \quad (3c)$$

$$P_C^n(x, t) = J_C'^n(x, t) + \gamma_C^n P_C^{n-1}(x, t) \quad (3d)$$

which are the conjugation of the gradient directions $J_k'^n$ and $J_C'^n$ at iteration n and the directions of descent P_k^{n-1} and P_C^{n-1} at iteration $n-1$ for k and C respectively. The conjugate coefficients are determined from

$$\gamma_k^n = \frac{\int_{x=0}^{1} \int_{t=0}^{t_f} (J_k'^n)^2 \, dt \, dx}{\int_{x=0}^{1} \int_{t=0}^{t_f} (J_k'^{n+1})^2 \, dt \, dx} \quad \text{with } \gamma_k^0 = 0 \quad (3e)$$

$$\gamma_C^n = \frac{\int_{x=0}^{1} \int_{t=0}^{t_f} (J_C'^n)^2 \, dt \, dx}{\int_{x=0}^{1} \int_{t=0}^{t_f} (J_C'^{n+1})^2 \, dt \, dx} \quad \text{with } \gamma_C^0 = 0. \quad (3f)$$

We note that when $\gamma^n = 0$ for any n, in equations (3e) and (3f), the direction of descent $P^n(x, t)$ becomes the gradient direction, i.e. the 'steepest-descent' method is obtained.

To perform the iterations according to equation (3), we need to compute the step sizes β_k^n and β_C^n and the gradient of the functional $J_k'^n$ and $J_C'^n$. In order to develop expressions for the determination of these quantities, the 'sensitivity problem' and 'adjoint problem' are constructed as described below.

5. SENSITIVITY PROBLEM AND SEARCH STEP SIZE

Since the problem involves two unknowns, in order to derive the sensitivity problem for each unknown, we should perturb the unknowns one at a time. It is assumed that when $k(x, t)$ undergoes a variation $\Delta k(x, t)$, $T(x, t)$ is perturbed by $T + \Delta T_k$. Then replacing k by $k + \Delta k$ and T by $T + \Delta T_k$ in the direct problem, and subtracting from the resulting expressions the direct problem and neglecting the second-order terms, the following sensitivity problems for the sensitivity function ΔT_k are obtained

$$\frac{\partial}{\partial x}\left(k(x, t)\frac{\partial \Delta T_k(x, t)}{\partial x}\right) + \frac{\partial}{\partial x}\left(\Delta k(x, t)\frac{\partial T(x, t)}{\partial x}\right) = C\frac{\partial \Delta T_k(x, t)}{\partial t} \quad \text{for } 0 < x < 1 \quad (4a)$$

$$-k(x, t)\frac{\partial \Delta T_k(x, t)}{\partial x} = \Delta k(x, t)\frac{\partial T(x, t)}{\partial x} \quad \text{for } x = 0 \quad (4b)$$

$$-k(x,t)\frac{\partial \Delta T_k(x,t)}{\partial x} = \Delta k(x,t)\frac{\partial T(x,t)}{\partial x} \quad \text{for } x = 1 \tag{4c}$$

$$\Delta T_k(x,t) = 0 \quad \text{for } t = 0. \tag{4d}$$

Similarly, the sensitivity problem for ΔT_C can be derived as

$$\frac{\partial}{\partial x}\left[k(x,t)\frac{\partial \Delta T_C(x,t)}{\partial x}\right] = \Delta C\frac{\partial T(x,t)}{\partial t} + C\frac{\partial \Delta T_C(x,t)}{\partial t} \quad \text{for } 0 < x < 1 \tag{5a}$$

$$\frac{\partial \Delta T_C(x,t)}{\partial x} = 0 \quad \text{for } x = 0 \tag{5b}$$

$$\frac{\partial \Delta T_C(x,t)}{\partial x} = 0 \quad \text{for } x = 1 \tag{5c}$$

$$\Delta T_C(x,t) = 0 \quad \text{for } t = 0. \tag{5d}$$

The functional $J(\hat{k}^{n+1}, \hat{C}^{n+1})$ for iteration $n+1$ is obtained by rewriting equation (2) as

$$J(\hat{k}^{n+1}, \hat{C}^{n+1}) = \int_{t=0}^{t_f} \sum_{i=1}^{m} [T_i(\hat{k}^n - \beta_k^n P_k^n, \hat{C}^n - \beta_C^n P_C^n) - Y_i]^2 \, dt \tag{6a}$$

where we replaced $\hat{k}^{n+1}$ and $\hat{C}^{n+1}$ by the expression given by equations (3a) and (3b). If temperature $T_i(\hat{k}^n - \beta_k^n P_k^n, \hat{C}^n - \beta_C^n P_C^n)$ is linearized by a Taylor expansion, equation (6a) takes the form

$$J(\hat{k}^{n+1}, \hat{C}^{n+1}) = \int_{t=0}^{t_f} \sum_{i=1}^{m} [T_i(\hat{k}^n, \hat{C}^n) - \beta_k^n \Delta T_i^n(P_k^n) - \beta_C^n \Delta T_i^n(P_C^n) - Y_i]^2 \, dt \tag{6b}$$

where $\Delta T_i^n(P_k^n) \equiv \Delta T_k^n(x_i, t)$ and $\Delta T_i^n(P_C^n) \equiv \Delta T_C^n(x_i, t)$, and $T_i(\hat{k}^n, \hat{C}^n)$ is the solution of the direct problem by using the estimates of $\hat{k}(x,t)$ and $\hat{C}(x,t)$ for exact $k(x,t)$ and $C(x,t)$ at $x = x_i$.

The sensitivity functions $\Delta T_i(P_k^n)$ and $\Delta T_i(P_C^n)$ are taken as the solutions of equations (4) and (5) at the measured positions $x = x_i$ by letting $\Delta k = P_k^n$ and $\Delta C = P_C^n$ respectively [17]. The search step sizes β_k^n and β_C^n are determined by minimizing the functional given by equation (6b) with respect to β_k^n and β_C^n respectively. Finally the following expression results:

$$\beta_k^n = \frac{(\bar{\bar{T}}_1 \bar{\bar{T}}_4 - \bar{\bar{T}}_3 \bar{\bar{T}}_5)}{(\bar{\bar{T}}_2 \bar{\bar{T}}_4 - \bar{\bar{T}}_5^2)} \tag{7a}$$

$$\beta_C^n = \frac{(\bar{\bar{T}}_2 \bar{\bar{T}}_3 - \bar{\bar{T}}_1 \bar{\bar{T}}_5)}{(\bar{\bar{T}}_2 \bar{\bar{T}}_4 - \bar{\bar{T}}_5^2)} \tag{7b}$$

where

$$\bar{\bar{T}}_1 = \int_{t=0}^{t_f} \sum_{i=1}^{m} (T_i^n - Y_i)\Delta T_i^n(P_k^n) \, dt \tag{8a}$$

$$\bar{\bar{T}}_2 = \int_{t=0}^{t_f} \sum_{i=1}^{m} [\Delta T_i^n(P_k^n)]^2 \, dt \tag{8b}$$

$$\bar{\bar{T}}_3 = \int_{t=0}^{t_f} \sum_{i=1}^{m} (T_i^n - Y_i)\Delta T_i^n(P_C^n) \, dt \tag{8c}$$

$$\bar{\bar{T}}_4 = \int_{t=0}^{t_f} \sum_{i=1}^{m} [\Delta T_i^n(P_C^n)]^2 \, dt \tag{8d}$$

$$\bar{\bar{T}}_5 = \int_{t=0}^{t_f} \sum_{i=1}^{m} \Delta T_i^n(P_k^n)\Delta T_i^n(P_C^n) \, dt. \tag{8e}$$

6. ADJOINT PROBLEM AND GRADIENT EQUATION

To derive the adjoint problem for $k(x,t)$, equation (1a) is multiplied by the Lagrange multiplier (or adjoint function) $\lambda(x,t)$ and the resulting expression is integrated over the time and corresponding space domains. Then the result is added to the right-hand side of equation (2) to yield the following expression for the functional $J[k(x,t), C(x,t)]$:

$$J[k(x,t), C(x,t)] = \int_{t=0}^{t_f} \sum_{i=1}^{m} (T_i - Y_i)^2 \, dt + \int_{x=0}^{1}\int_{t=0}^{t_f} \lambda\left[\frac{\partial}{\partial x}\left(k(T)\frac{\partial T(x,t)}{\partial x}\right) - C\frac{\partial T(x,t)}{\partial t}\right] dt\, dx. \tag{9}$$

The variation ΔJ_k is obtained by perturbing T by ΔT_k in equation (9), subtracting from the resulting expression the original equation (9) and neglecting the second-order terms. We thus find

$$\begin{aligned}\Delta J_k = {} & 2\int_{t=0}^{t_f} (T_1 - Y_1)\Delta T_1(P_k) \, dt + 2\int_{t=0}^{t_f} (T_m - Y_m)\Delta T_m(P_k) \, dt \\ & + 2\int_{x=0}^{1}\int_{t=0}^{t_f} \sum_{i=2}^{m-1} (T - Y)\Delta T(P_k)\delta(x - x_i) \, dt\, dx \\ & + \int_{x=0}^{1}\int_{t=0}^{t_f} \lambda\left[\frac{\partial}{\partial x}\left(k(x,t)\frac{\partial \Delta T_k(x,t)}{\partial x}\right) + \frac{\partial}{\partial x}\left(\Delta k(x,t)\frac{\partial T(x,t)}{\partial x}\right) - C\frac{\partial \Delta T_k(x,t)}{\partial t}\right] dt\, dx\end{aligned} \tag{10}$$

where $\delta(x - x_i)$ is the Dirac delta function and x_i, $i = 2$ to $m-1$, refer to the internal measured positions. In equation (10), the second double integral term is integrated by parts; the initial and boundary conditions of the sensitivity problem given by equations (4b)–(4d) are utilized and then ΔJ_k is allowed to go to zero.

The vanishing of the integrands containing ΔT_k leads to the following adjoint problem for the determination of $\lambda(x,t)$:

$$\frac{\partial}{\partial x}\left[k(x,t)\frac{\partial \lambda(x,t)}{\partial x}\right]+\sum_{i=2}^{m-1}2(T-Y)\delta(x-x_i)+\frac{\partial[C(x,t)\lambda(x,t)]}{\partial t}=0 \quad \text{for } 0<x<1 \tag{11a}$$

$$-k(x,t)\frac{\partial \lambda(x,t)}{\partial x}=2(T_1-Y_1) \quad \text{for } x=0 \tag{11b}$$

$$k(x,t)\frac{\partial \lambda(x,t)}{\partial x}=2(T_m-Y_m) \quad \text{for } x=1 \tag{11c}$$

$$\lambda(x,t)=0 \quad \text{for } t=t_f. \tag{11d}$$

This adjoint problem is different from the standard initial value problems in that the final time condition at time $t=t_f$ is specified instead of the customary initial condition. However, this problem can be transformed to an initial value problem by the transformation of the time variables as $\tau=t_f-t$. Then standard techniques can be used to solve the above adjoint problem.

Finally, the following integral term is left

$$\Delta J_k=\int_0^1\int_{t=0}^{t_f}-\left[\frac{\partial \lambda(x,t)}{\partial x}\frac{\partial T(x,t)}{\partial x}\right]\Delta k(x,t)\,dt\,dx \tag{12a}$$

For $k=k(x,t)\in L_{2\text{-norm}}$, $x\in[0,1]$ and $t\in[0,t_f]$, from the definition used in [10], we have

$$\Delta J_k=\int_0^1\int_{t=0}^{t_f}J'_k(x,t)\Delta k(x,t)\,dt\,dx. \tag{12b}$$

Then the function $J'_k(x,t)$ is called a gradient of functional for determining $k(x,t)$. A comparison of equations (12a) and (12b) leads to the following expression for the gradient $J'_k(x,t)$ of the functional J:

$$J'_k(x,t)=-\frac{\partial \lambda(x,t)}{\partial x}\frac{\partial T(x,t)}{\partial x}. \tag{12c}$$

Similarly, to derive the adjoint problem for $C(x,t)$, equation (1a) is multiplied by the Lagrange multiplier (or adjoint function) $\Lambda(x,t)$ and the same procedure as described before is followed. Eventually we find that the adjoint equation for estimating C is identical to the adjoint equation for estimating k [15]; this implies that the adjoint equations need to be solved only once, since $\lambda=\Lambda$. Finally the gradient equation of the functional for determining $C(x,t)$ can be obtained as

$$J'_C(x,t)=-\lambda(x,t)\frac{\partial T(x,t)}{\partial t}. \tag{12d}$$

We note that $J'(x,t_f)$ always equals zero since $\lambda(x,t_f)=0.0$, therefore if the final time values of $k(x,t_f)$ and $C(x,t_f)$ cannot be predicted before the inverse calculation, the estimated values of $k(x,t)$ and $C(x,t)$ will deviate from the exact values near the final time condition [10]. This is the case in the present study! Generally speaking, there are two methods to avoid such a singularity, one is to use the modified conjugate gradient method [11] and the other one is to record data a little longer than the actual period of interest.

However, in the present study we find an alternative method to satisfy this requirement, i.e. if we let $\lambda(x,t_f)=\lambda(x,t_f-\Delta t)\neq 0$, where Δt denotes the time increment for use in the finite-difference calculation, the singularity at $t=t_f$ can be avoided and a reliable inverse solution can be obtained. We should note that the above-stated approach might only be good for this specific problem, since it relates strongly to the form of the gradient equation!

7. STOPPING CRITERION

If the problem contains no measurement errors, the traditional check condition is specified as

$$J[\hat{k}^{n+1}(x,t),\hat{C}^{n+1}(x,t)]<\varepsilon \tag{13}$$

where ε is a small specified number. However, the observed temperature data will contain measurement errors. Therefore, we do not expect the functional equation (2) to be equal to zero at the final iteration step. Following the experience of the authors [10–15], we use the discrepancy principle as the stopping criterion, i.e. we assume that the temperature residuals may be approximated by

$$T_i-Y_i\approx\sigma \tag{14}$$

where σ is the standard deviation of the measurements and is assumed to be a constant. The above assumption was also made by Tikhonov and Arsenia [18] in order to find the optimal regularization parameter. Substituting equation (14) into equation (2), the following expression is obtained for ε:

$$\varepsilon=m\sigma^2t_f. \tag{15}$$

Then, the stopping criterion is given by equation (13) with ε determined from equation (15).

8. RESULTS AND DISCUSSIONS

To illustrate the validity and accuracy of the conjugate gradient method in simultaneously predicting $k(T)$ and $C(T)$ with inverse analysis from the knowledge of transient temperature recordings, we consider a specific example where the exact functional form of thermal conductivity is assumed to be the combination of the sinusoidal and exponential functions while heat capacity per unit volume is taken as a second-order polynomial with temperature as the dependent variable, i.e.

$$k(T) = K_0 + K_1 \times \exp\left(\frac{T}{K_2}\right) + K_3 \times \sin\left(\frac{T}{K_4}\right) \quad (16a)$$

$$C(T) = C_0 + C_1 \times T + C_2 \times T^2 \quad (16b)$$

where the constants K_0, K_1, K_2, K_3 and K_4 for $k(T)$ are taken as 1, 4.5, 80, 2.5 and 3 respectively, and the constants C_0, C_1 and C_2 for $C(T)$ are chosen as 1.2, 0.02 and 0.00001, respectively. The material has initial temperature $T_0 = 1$, when $t > 0$, and two boundaries are subjected to a constant heat flux, $q_1 = 17$ and $q_2 = 6$ respectively. The exact functions for $k(T)$ and $C(T)$ in terms of $k(x, t)$ and $C(x, t)$ within the total space and time domain are sketched in Figs. 2(a) and 2(b), respectively. The objective of this article is to show the applicability of the present approach in measuring $k(T)$ and $C(T)$ accurately with no prior information on the functional form of the unknown quantities, which is the so-called function estimation.

In order to compare the results for situations involving random measurement errors, we assume normally distributed uncorrelated errors with zero mean and constant standard deviation. The simulated inexact measurement data Y can be expressed as

$$Y = Y_{\text{exact}} + \omega\sigma \quad (17)$$

where Y_{exact} is the solution of the direct problem with the exact values of $k(T)$ and $C(T)$; σ is the standard deviation of the measurements; and ω is a random variable that is generated by subroutine DRNNOR of the IMSL [19] and will be within -2.576 to 2.576 for a 99% confidence bounds. One should note that, when generating simulated measurement temperature Y, exact $k(T)$ and $C(T)$ are used in the direct problem and thus the problem is nonlinear and the iterative technique is needed for its solutions. However, in the inverse calculation, the thermal conductivity and heat capacity exist in the form of $k(x, t)$ and $C(x, t)$, so the problem becomes linear and the estimated temperature can be calculated directly.

The space and time increments are taken as $\Delta x = 0.1$ and $\Delta t = 0.02$ respectively, in the finite-difference calculations; the total measurement time is chosen as $t_f = 1.2$; thermocouple spacing Dx equals the finite-difference spacing Δx and measurement time step Dt is taken the same as Δt, therefore a total of 660 discrete numbers of $k(x, t)$ and 660 discrete numbers of $C(x, t)$ are to be estimated simultaneously in the inverse calculations. We now present below the numerical experiments in simultaneously determining $k(T)$ and $C(T)$ by the inverse analysis.

One of the advantages of using the conjugate gradient method is that the initial guesses of the unknown quantities can be chosen arbitrarily. However, this is not valid in the present study. The reason is because two unknown functions, $k(x, t)$ and $C(x, t)$, are to be estimated simultaneously by using only the measurement temperature $Y(x, t)$, which implies that the estimated temperature $T(x, t)$ obtained by utilizing any combination of $k(x, t)$ and $C(x, t)$ could possibly equal $Y(x, t)$, but the estimated thermal properties are not the correct ones.

In order to restrict the region of search directions to obtain the correct inverse solutions, a good initial guess of either thermal conductivity, $k(x, t)$, or heat capacity, $C(x, t)$, should be given prior to the inverse calculations. Fortunately, good initial guesses for heat capacity, $\hat{C}^0(x, t)$, can be obtained from the following energy balance equation

$$[q(t_{j+1}) - q(t_j)]\Delta t = \int_{x=0}^{x=1} \tilde{C}(t_j)[T(x, t_{j+1}) - T(x, t_j)]\,dx \quad (18)$$

where $q = q_1 - q_2$; j represents the time index; Δt denotes the time increment for use in the finite-difference calculation and $\tilde{C}(t_j)$ is an averaged value for heat capacity at $t = t_j$. Therefore good initial guesses for heat capacity are obtained as $\hat{C}^0(x, t) = \tilde{C}(t)$.

Once good initial guesses of heat capacity are obtained, the procedure for the inverse calculation can be as follows. Firstly, by fixing this good initial guess of heat capacity, $\hat{C}^0(x, t)$, the thermal conductivity, $\hat{k}(x, t)$, with any arbitrary initial guess can be calculated to approach the exact $k(x, t)$ in the inverse algorithm within a few iterations. Secondly, by using those good but not accurate values of $\hat{k}(x, t)$ and $\hat{C}(x, t)$ in the conjugate gradient method, the thermal properties can be refined and accurate inverse solutions for $k(x, t)$ and $C(x, t)$ are thus obtained. In all the test cases considered here, the initial guesses of $\hat{k}(x, t)$ used to begin the iteration are taken as $\hat{k}^0(x, t) = 10^{-8}$.

The estimated functions of $k(x, t)$ and $C(x, t)$, obtained when using exact measurements, $\sigma = 0.0$, are shown in Figs. 3(a) and 3(b) respectively. The value of functional J obtained in such a case can be decreased to a very small number as the number of iterations is increased. The comparison between Figs. 2 and 3 shows that the inverse analysis with the conjugate gradient method in simultaneously measuring $k(x, t)$ and $C(x, t)$ is now accomplished.

Next, the dimensionless measured temperature with errors $\sigma = 0.001$ and $\sigma = 0.005$ are obtained according to equation (17) which represent a maximum temperature rise of about 0.02% and 0.1% respectively. The inverse solutions using these inexact measurements as the simulated temperature measurements are shown in Figs. 4 and 5, respectively. In order to show $k(T)$ and $C(T)$ more explicitly as functions of temperature, T, the thermal conductivity and heat capacity per unit volume at $x = 0.5$ with measurement errors $\sigma = 0$, 0.001 and 0.005 are presented in Figs. 6(a) and 6(b) respectively. As expected, increases in the measurement errors cause decreases in the accuracy of the inverse solution.

The average relative error between the exact and estimated values for $k(x, t)$ and $C(x, t)$ are listed in Table 1 and such an error is defined as

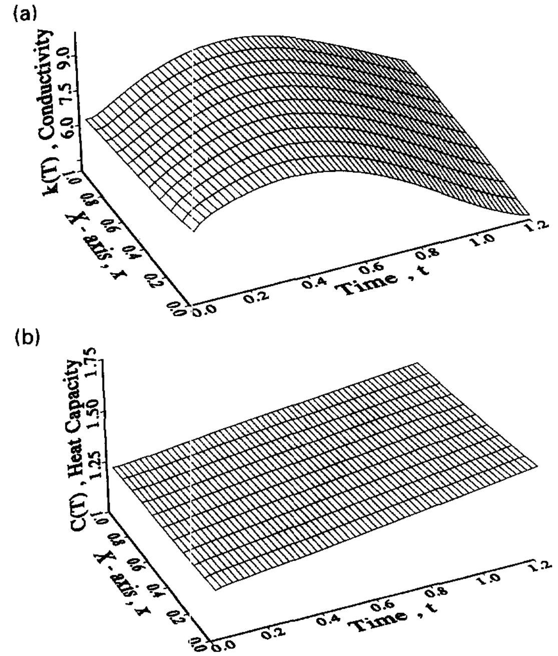


Fig. 2. (a) The exact function of $k(T)$; (b) the exact function of $C(T)$.

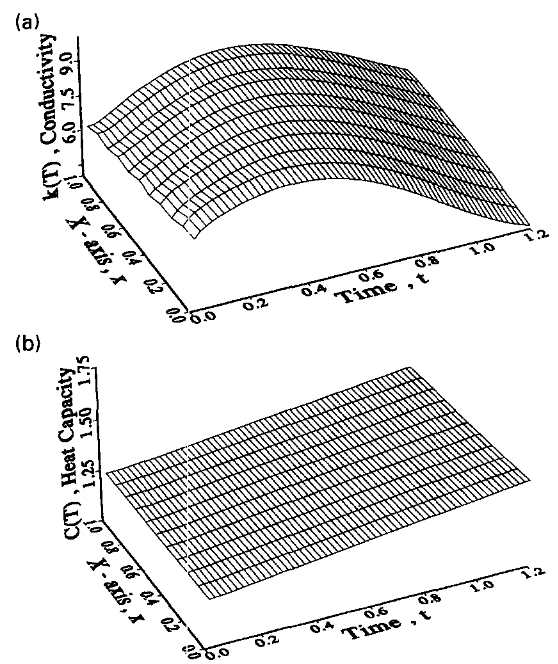


Fig. 3. (a) The estimated function of $k(T)$ with $\sigma = 0.0$; (b) the estimated function of $C(T)$ with $\sigma = 0.0$.

$$k_{\text{error}} = \left(\sum_{i=1}^{m} \sum_{j=1}^{n} \left| \frac{k(x_i, t_j) - \hat{k}(x_i, t_j)}{k(x_i, t_j)} \right| \right) \Big/ (n \times m) \times 100\% \tag{19a}$$

$$C_{\text{error}} = \left(\sum_{i=1}^{m} \sum_{j=1}^{n} \left| \frac{C(x_i, t_j) - \hat{C}(x_i, t_j)}{C(x_i, t_j)} \right| \right) \Big/ (n \times m) \times 100\% \tag{19b}$$

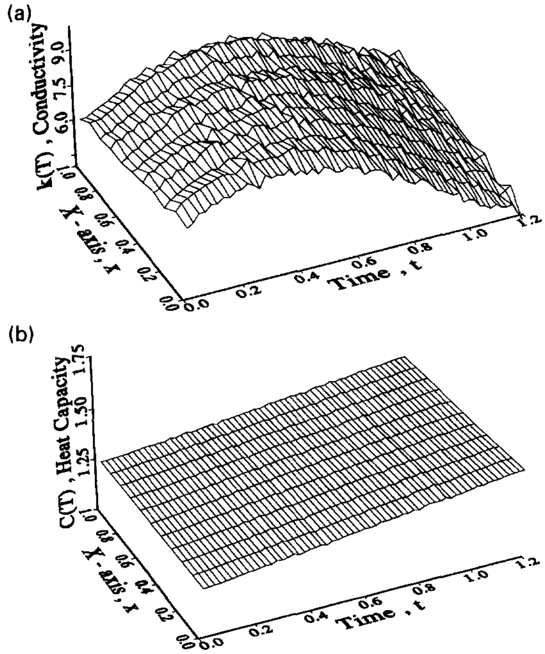


Fig. 4. (a) The estimated function of $k(T)$ with $\sigma = 0.001$; (b) the estimated function of $C(T)$ with $\sigma = 0.001$.

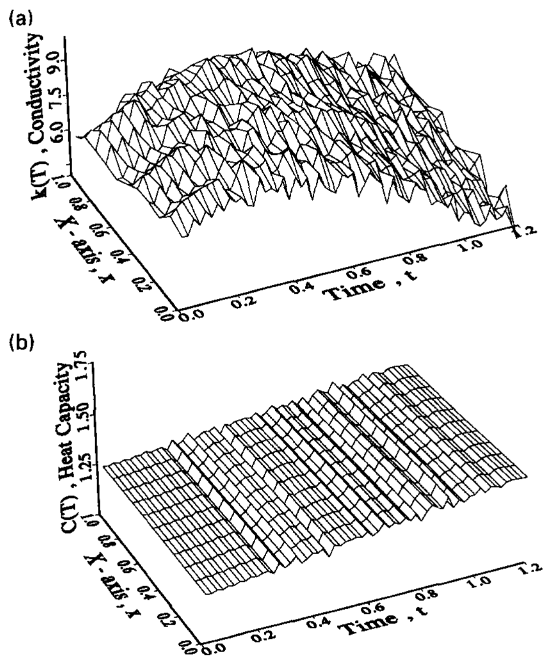


Fig. 5. (a) The estimated function of $k(T)$ with $\sigma = 0.005$; (b) the estimated function of $C(T)$ with $\sigma = 0.005$.

where m and n represent the total discrete number of position and time increments, respectively. Table 1 also shows the number of iterations and CPU time used on a VAX-9420 computer for simultaneously measuring $k(x, t)$ and $C(x, t)$. Indeed, the necessary CPU time is within 1.4 and 4.46 s in estimating 660 unknown discrete numbers of $k(x, t)$ and 660 unknown discrete numbers of $C(x, t)$, this shows that the speed of convergence is very fast!

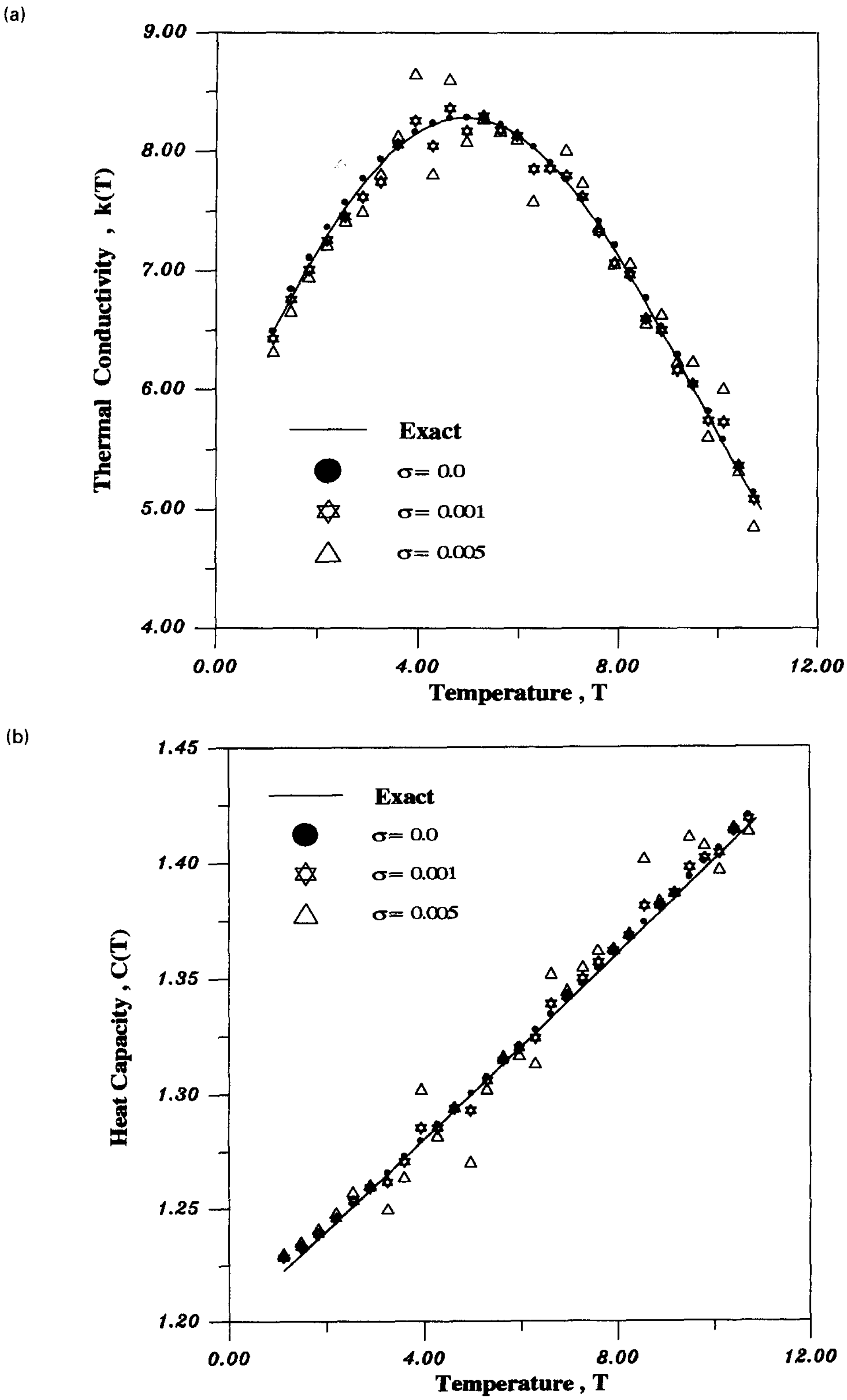


Fig. 6. (a) The exact and estimated values of $k(T)$ at $x = 0.5$; (b) the exact and estimated values of $C(T)$ at $x = 0.5$.

Table 1. The convergent parameters of the inverse problem

Case: $k(T) = K_0 + K_1 \times \exp(T/K_2) + K_3 \times \sin(T/K_4)$; $C(T) = C_0 + C_1 \times T + C_2 \times T^2$

Measurement error, σ	Stop criterion	Number of iterations	VAX-9420 CPU time (s)	Average relative error %	
				C_{error}	k_{error}
0.000	1.00 E-008	148	4.46	0.69	0.510
0.001	1.32 E-005	57	2.28	0.706	1.502
0.005	3.20 E-004	26	1.40	1.026	4.101

9. CONCLUSIONS

The conjugate gradient method with the adjoint equation was successfully applied for the solution of the inverse problem to determine simultaneously the temperature-dependent thermal conductivity, $k(T)$ and heat capacity per unit volume, $C(T)$. Several test cases involving different measurement errors were considered. The results show that the conjugate gradient method does not require *a priori* information for the functional forms of the unknown quantities and needs very short CPU time on a VAX-9420 to perform the inverse calculations.

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