A direct integration approach for simultaneously estimating spatially varying thermal conductivity and heat capacity

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One of the difficulties in the solution of inverse heat conduction problems is that of making sufficiently accurate initial guesses of the unknowns in order to start the iterations. In this work a direct integration methodology is developed for determining good initial guesses for the unknown property coefficients. Having good initial guesses, the analyst can apply the Levenberg–Marquardt method to refine the results to within a specified convergence criteria.

The problem studied here is concerned with simultaneous estimation of spatially varying thermal conductivity and heat capacity from multiple spatial and temporal measurements made during transient heat conduction. Interior temperature sensors are necessary when the properties vary spatially. A statistical analysis is performed to determine approximate confidence bounds for estimating the thermal conductivity and heat capacity per unit volume.

Keywords: inverse conduction; property determination; transient conduction

Introduction

This work addresses development of an efficient method of analysis for estimating simultaneously the thermal conductivity, k, and heat capacity per unit volume, ρC_p, that vary linearly and continuously with distance in the direction normal to the sample, using multiple spatial and temporal temperature measurements in transient heat conduction experiments.

One of the drawbacks of the existing methods of inverse analysis is that there is no way for making sufficiently accurate initial guesses to start the calculations. Thus a large number of iterations are needed for convergence, and sometimes the solutions never converge. In order to alleviate such difficulties, we developed a new expression to use in making sufficiently accurate initial guesses.

Reports of inverse heat conduction analyses that deal with simultaneous determination of spatially varying thermal conductivity and heat capacity are limited in the literature. Ciampi *et al.*[1] proposed an approximate direct solution applicable to slightly heterogeneous samples for use with flash-type experiments, utilizing temporal temperature measurements made only at the insulated back surface of the slab sample. They considered linear and exponential variations with distance of thermal conductivity and heat capacity per unit volume; they never examined simultaneous estimation of thermal conductivity and heat capacity.

Numerous engineering and mathematical researchers have considered problems equivalent to estimating spatially dependent thermal conductivity alone. These include researchers Carotenuto *et al.*,[2] Kubrusly and Curtain,[3] Travis and White,[4] Carotenuto and Raiconi,[5] Liu and Chen,[6] Chen and Liu,[7] Alt *et al.*,[8] Kravaris and Seinfeld,[9] Liu and Chen,[10] Kitamura and Nakagiri,[11] and Chen and Seinfeld.[12] Determination of spatially dependent thermal properties is a special case of a general class of mathematical problems called *distributed parameter system* problems. Ray[13] lists applications of distributed parameter system theory to numerous physical problems. Kubrusly,[14] Tzafestas and Stavroulakis,[15] Goodson and Polis,[16] and Raibman *et al.*[17] give reviews and surveys of the distributed parameter system literature.

Flach and Özişik[18] developed parameters for the unknown thermal properties with piecewise linear spline representation in the space variable and applied the least squares method to determine the two properties simultaneously. Their analysis required a considerable amount of computer time because of the difficulties in making sufficiently accurate initial guesses.

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Problem formulation

To illustrate the method for developing expressions to use in determining sufficiently accurate estimates for the unknown property coefficients, we present the following transient inverse heat conduction problem. A slab of thickness L is initially at zero temperature. For time >0, the boundary surface at $x=L$ is kept insulated, while that at $x=0$ is subjected to a prescribed heat flux of strength q W/m^2. The mathematical model of this one-dimensional (1-D) transient heat conduction problem is

$$\frac{\partial}{\partial x}\left[k(x)\frac{\partial T(x,t)}{\partial x}\right]=C(x)\frac{\partial T(x,t)}{\partial t} \tag{1a}$$

$$-k(0)\frac{\partial T(0,t)}{\partial x}=q \tag{1b}$$

$$\frac{\partial T(L,t)}{\partial x}=0 \tag{1c}$$

$$T(x,0)=0 \tag{1d}$$

where $C(x)=\rho Cp(x)$ is the heat capacity per unit volume. We assume that temperature sensors are installed at the spatial positions, x_i $(i=0,1,2,\ldots,N)$, in the slab, with x_0 representing the left boundary and x_N representing the right boundary. Temperature readings are taken at each of these spatial positions at times t_j $(j=0,1,2,\ldots,M)$. Thus a total of $(M+1)\times$

$(N+1)\equiv\Omega$ measurements are available. The inverse heat conduction problem posed here is as follows: Utilizing Ω measurement data—taken within the medium as well as at the boundary surfaces—we determine the thermal properties $k(x)$ and $C(x)$, assuming that these properties vary linearly and continuously in the direction normal to the sample plate.

Direct solution of the problem

The first step in the inverse analysis is development of the corresponding direct solution for the problem (Equations 1). Any one of several well-established analytical or numerical approaches can be used to solve the problem. Here we consider the weighted finite difference method, using a weight factor of $0\leq\theta\leq 1$ and uniform space grids. The resulting finite difference equations, in matrix form, are

$$\begin{bmatrix} b_0 & c_0 & 0 & \cdots & & 0 \\ a_1 & b_1 & c_1 & 0 & & \vdots \\ 0 & & & & & 0 \\ \vdots & & 0 & a_{N-1} & b_{N-1} & c_{N-1} \\ 0 & \cdots & & 0 & a_N & b_N \end{bmatrix} \begin{bmatrix} T_0 \\ T_1 \\ \vdots \\ T_{N-1} \\ T_N \end{bmatrix} = \begin{bmatrix} d_0 \\ d_1 \\ \vdots \\ d_{N-1} \\ d_N \end{bmatrix} \tag{2a}$$

where

$$a_i=\frac{\theta[k(x_i)+k(x_{i-1})]}{2\Delta x} \qquad i=1,2,\ldots,N \tag{2b}$$

$$c_i=\frac{\theta[k(x_{i+1})+k(x_i)]}{2\Delta x} \qquad i=0,1,\ldots,N-1 \tag{2c}$$

$$b_i=-\left[\frac{\theta[k(x_{i+1})+2k(x_i)+k(x_{i-1})]}{2\Delta x}+\frac{C(x_i)\,\Delta x}{\Delta t}\right] \qquad i=1,2,\ldots,N-1 \tag{2d}$$

$$b_0=-\left[\frac{\theta[k(x_1)+k(x_0)]}{2\Delta x}+\frac{C(x_0)\,\Delta x}{2\Delta t}\right] \tag{2e}$$

$$b_N=-\left[\frac{\theta[k(x_N)+k(x_{N-1})]}{2\Delta x}+\frac{C(x_N)\,\Delta x}{2\Delta t}\right] \tag{2f}$$

$$d_i=-\frac{(1-\theta)[k(x_i)+k(x_{i-1})]}{2\Delta x}T_{i-1}^n+\left[\frac{(1-\theta)[k(x_{i+1})+k(x_i)+k(x_{i-1})]}{2\Delta x}-\frac{C(x_i)\,\Delta x}{\Delta t}\right]T_i^n-\frac{(1-\theta)[k(x_{i+1})+k(x_i)]}{2\Delta x}T_{i+1}^n \qquad i=1,2,\ldots,N-1 \tag{2g}$$

$$d_0=-\left[\frac{(1-\theta)[k(x_1)+k(x_0)]}{2\Delta x}-\frac{C(x_0)\,\Delta x}{2\Delta t}\right]T_0^n-\frac{(1-\theta)[k(x_1)+k(x_0)]}{2\Delta x}T_1^n-\theta q^{n+1}-(1-\theta)q^n \tag{2h}$$

$$d_N=-\frac{(1-\theta)[k(x_N)+k(x_{N-1})]}{2\Delta x}T_{N-1}^n+\left[\frac{(1-\theta)[k(x_N)+k(x_{N-1})]}{2\Delta x}-\frac{C(x_N)\,\Delta x}{2\Delta t}\right]T_N^n \tag{2i}$$

where the weight θ chosen is $\frac{2}{3}$, which is Galerkin weighting. At each time level n, the tridiagonal matrix in Equation 2 is solved using the Thomas algorithm.

Inverse analysis by direct integration

We now present a method for developing an expression to use in making sufficiently accurate first estimates for $k(x)$ and $C(x)$, utilizing the temperature measurements made with sensors at $N+1$ locations and at $M+1$ times. Figure 1 illustrates the locations $x_0, x_1, \ldots, x_N$ of the sensors, where x_0 and x_N are the left and right boundary surfaces, respectively.

The basic steps in the analysis are as follows. We integrate Equation 1a twice with respect to x and once with respect to t:

$$\int_0^{t_j}\int_{x_0}^{x_i}\int_{x_0}^{x}\frac{\partial}{\partial x'}\left[k(x')\frac{\partial T(x',t)}{\partial x'}\right]dx'\,dx\,dt=\int_{x_0}^{x_i}\int_{x_0}^{x}\int_0^{t_j}C(x')\frac{\partial T(x',t)}{\partial t}\,dt\,dx'\,dx \tag{3}$$

Next, we perform the integration with respect to x' on the left-hand side and the integration with respect to t on the right-hand side of Equation 3:

$$\int_0^{t_j}\int_{x_0}^{x_i}\left[k(x)\frac{\partial T(x,t)}{\partial x}-k(x_0)\left(\frac{\partial T(x,t)}{\partial x}\right)_{x=x_0}\right]dx\,dt=\int_{x_0}^{x_i}\int_{x_0}^{x}C(x')[T(x',t_j)-T(x',t_0)]\,dx'\,dx \tag{4}$$

We then integrate the first term on the left-hand side of Equation 4

Figure 1 Location of sensors

Notation

$C(x)$	Heat capacity per unit volume, $\rho C_p(x)$
C_0, C_N	Heat capacity coefficients
$C_p(x)$	Specific heat capacity
$E(\bullet)$	Expected value operator
$k(x)$	Thermal conductivity
K_0, K_N	Thermal conductivity coefficients
L	Slab thickness
$\hat{\mathbf{P}}$	Vector of estimated parameters, K_0, K_N, C_0, and C_N
q	Total heat input at surface $x=0$
t	Time
$T(x, t)$	Interior temperature
var–cov($\bullet$)	Variance–covariance matrix
x	Spatial coordinate

Greek symbols

θ	Weight factor
ρ	Density
σ	Standard deviation
Ω	Total number of measurements, $(M+1)\times(N+1)$

Superscripts

$\hat{}$	Estimated quantity
$\tilde{}$	Measured quantity

with respect to x by parts:

$$\int_{x_0}^{x_i} k(x)\frac{\partial T(x,t)}{\partial x}\,dx \equiv k(x_i)T(x_i,t) - k(x_0)T(x_0,t) - \int_{x_0}^{x_i}\frac{\partial k(x)}{\partial x}T(x,t)\,dx \tag{5a}$$

and apply the Cauchy integral formula to the right-hand side of Equation 4:

$$\int_{x_0}^{x_i}\int_{x_0}^{x} C(x')[T(x',t_j)-T(x',t_0)]\,dx'\,dx \equiv \int_{x_0}^{x_i}(x_i-x)C(x)[T(x,t_j)-T(x,t_0)]\,dx \tag{5b}$$

We substitute the resulting expressions, Equations 5a and 5b into Equation 4 to obtain

$$\int_0^{t_j} k(x_i)T(x_i,t)\,dt - \int_0^{t_j} k(x_0)T(x_0,t)\,dt - \int_0^{t_j}\int_{x_0}^{x_i}\frac{\partial k(x)}{\partial x}T(x,t)\,dx\,dt - \int_0^{t_j} k(x_0)\left(\frac{\partial T(x,t)}{\partial x}\right)_{x=x_0}(x_i-x_0)\,dt = \int_{x_0}^{x_i}(x_i-x)C(x)T(x,t)\,dx \tag{6}$$

where x_0 and x_N refer to the boundary sensors and x_i $(i=1,2,\ldots,N-1)$ refer to the interior sensors. We eliminate the last term on the left-hand side of Equation 6 in the following manner. We set $i=N$ in Equation 6 and multiply the resulting expression by (x_i-x_0) then multiply Equation 6 by (x_N-x_0) and subtract the two results. We obtain

$$\begin{aligned}
&(x_i-x_0)k(x_N)\int_0^{t_j} T(x_N,t)\,dt - (x_N-x_0)k(x_i)\int_0^{t_j} T(x_i,t)\,dt \\
&+(x_Nn-x_i)k(x_0)\int_0^{t_j} T(x_0,t)\,dt \\
&+(x_N-x_i)\int_0^{t_j}\int_{x_0}^{x_i}\frac{\partial k(x)}{\partial x}T(x,t)\,dx\,dt \\
&-(x_i-x_0)\int_0^{t_j}\int_{x_i}^{x_N}\frac{\partial k(x)}{\partial x}T(x,t)\,dx\,dt \\
&+(x_N-x_i)\int_{x_0}^{x_i}(x_0-x)C(x)T(x,t)\,dx \\
&-(x_i-x_0)\int_{x_i}^{x_N}(x_N-x)C(x)T(x,t_j)\,dx = 0
\end{aligned} \tag{7}$$

An additional relation can be determined by considering a gross energy balance over the slab from $x=x_0$ to $x=x_N$. We consider the case of constant heat flux q W/m^2, releasing its energy continuously at the boundary surface $x=x_0$, while the boundary at $x=x_N$ is kept insulated. The energy balance gives

$$\int_0^{t_j} q\,dt = qt_j = \int_0^{x_N} C(x)[T(x,t_j)-T(x,t_0)]\,dx \tag{8}$$

where $T(x,t_0)$ is the initial condition.

If temperature measurements are made at every one of the $N+1$ sensors at each time, Equation 7 for $i=1$ to $N-1$ provides $N-1$ independent relations, and Equation 8 provides an additional relation. If the problem involves η unknown coefficients, then measurements should be made at least for $j \geqq \mathrm{INT}(\eta/N)$ different times, where INT(●) refers to the larger value of the integer. We now examine a situation in which properties $k(x)$ and $C(x)$ vary linearly with x.

Properties varying linearly in space

Let $k(x)$ and $C(x)$ vary linearly with the space coordinate normal to the plate. We consider two sensors placed inside the medium (x_1 and x_2) and two sensors at the boundary surfaces (x_0 and x_3), as illustrated in Figure 2. The problem involves four unknown property coefficients which we choose at their boundary values, that is, K_0, K_3, C_0, and C_3. We can conveniently express $k(x)$ and $C(x)$ in terms of these coefficients:

$$k(x) = \frac{K_3-K_0}{x_3-x_0}(x-x_0)+K_0 \tag{9a}$$

and

$$C(x) = \frac{C_3-C_0}{x_3-x_0}(x-x_0)+C_0 \tag{9b}$$

Then their derivatives become

$$\frac{\partial k(x)}{\partial x} = \frac{K_3-K_0}{x_3-x_0} \quad\text{and}\quad \frac{\partial C(x)}{\partial x} = \frac{C_3-C_0}{x_3-x_0} \tag{9c,d}$$

We substitute Equations 9 into Equation 7 and rearrange the result in the form:

$$K_0Y_0 + K_3Y_3 + C_0Z_0 + C_3Z_3 = 0 \tag{10a}$$

where

$$Y_0 = \left\{(x_i-x_3)\int_0^{t_j} T(x_i,t)\,dt + (x_3-x_i)\int_0^{t_j} T(x_0,t)\,dt - \frac{x_3-x_i}{x_3-x_0}\int_0^{t_j}\int_{x_0}^{x_i} T(x,t)\,dx\,dt + \frac{x_i-x_0}{x_3-x_0}\int_0^{t_j}\int_{x_i}^{x_3} T(x,t)\,dx\,dt\right\} \tag{10b}$$

$$Y_3 = \left\{(x_i-x_0)\int_0^{t_j} T(x_3,t)\,dt - (x_i-x_0)\int_0^{t_j} T(x_i,t)\,dt + \frac{x_3-x_i}{x_3-x_0}\int_0^{t_j}\int_{x_0}^{x_i} T(x,t)\,dx\,dt - \frac{x_i-x_0}{x_3-x_0}\int_0^{t_j}\int_{x_i}^{x_3} T(x,t)\,dx\,dt\right\} \tag{10c}$$

$$\begin{aligned}
Z_0 = \Bigg\{&\frac{x_i-x_3}{x_3-x_0}\int_{x_0}^{x_i}(x_0-x)(x-x_0)T(x,t_j)\,dx \\
&+\frac{x_i-x_0}{x_3-x_0}\int_{x_i}^{x_3}(x_3-x)(x-x_0)T(x,t_j)\,dx \\
&+(x_3-x_i)\int_{x_0}^{x_i}(x_0-x)T(x,t)\,dx \\
&-(x_i-x_0)\int_{x_i}^{x_3}(x_3-x)T(x,t_j)\,dx\Bigg\}
\end{aligned} \tag{10d}$$

Figure 2 Application of linearly varying properties

$$Z_3=\left\{\frac{x_3-x_i}{x_3-x_0}\int_{x_0}^{x_i}(x_0-x)(x-x_0)T(x,t_j)\,dx - \frac{x_i-x_0}{x_3-x_0}\int_{x_i}^{x_3}(x_3-x)(x-x_0)T(x,t_j)\,dx\right\} \tag{10e}$$

We substitute Equations 9 into Equation 8, assuming that the heat flux q is constant. We obtain

$$C_0W_0+C_3W_3=qt_j \tag{11a}$$

where

$$W_0=\left\{\frac{-1}{x_3}\int_0^{x_3}xT(x,t_j)\,dx+\int_0^{x_3}T(x,t_j)\,dx\right\} \tag{11b}$$

$$W_3=\left\{\frac{1}{x_3}\int_0^{x_3}xT(x,t_j)\,dx\right\} \tag{11c}$$

Thus, for each time step t_j, we can obtain two relations from Equation 10 by setting $i=1$ and 2 and one additional relation from the energy balance equation, Equation 11. The problem involves four unknowns, so at least two time measurements are needed. This procedure provides an overdetermined system, with at least six simple algebraic equations for determining the four unknown property coefficients to be used as first guesses to start the iterations for the inverse analysis. This overdetermined system of equations can be solved by IMSL subroutine DLSBRR,[19] which utilizes the least squares method to solve the system of equations.

Refinement of the inverse solution

The method developed provides us with sufficiently accurate initial guesses for the unknown parameters, which we now use in the inverse analysis as initial guesses. We consider the sum of the least square norm, S:

$$S(\hat{P}_j)=\sum_{i=1}^{\Omega}(\tilde{T}_i-\hat{T}_i(\hat{P}_j))^2 \qquad j=1,2,3,\text{ and }4 \tag{12}$$

where Ω is the total number of temperature measurements and $\hat{T}_i(\hat{P}_j)$ are the temperatures obtained from the direct solution of the problem (Equation 1) by using the estimated values of the four unknown parameters $\hat{\mathbf{P}}\equiv K_0, K_3, C_0, C_3\}$. Equation 12 is minimized with respect to the estimated parameters $\hat{\mathbf{P}}$:

$$\sum_{i=1}^{\Omega}\left(\frac{\partial\hat{T}_i}{\partial\hat{P}_j}\right)(\tilde{T}_i-\hat{T}_i)=0 \qquad j=1,2,3,\text{ and }4 \tag{13}$$

Because this system is nonlinear, an iterative technique is necessary for its solution. We chose the modified Levenberg–Marquardt algorithm, available in IMSL Library Edition 10.0 as subroutine DBCLSJ[19] to solve the nonlinear least squares Equation 13. The procedure developed provided excellent initial guesses to start the iterations. The program computes the Jacobian matrix, $\partial\hat{T}_i/\partial\hat{P}_j$, that appears in Equation 13, with forward finite differences. Bounds are specified for the parameters $\hat{\mathbf{P}}$ between zero and a large positive number, as all the thermal properties must be positive.

Statistical analysis

Statistical analysis is important in determining the accuracy of the computed inverse solution. Here, we develop confidence bounds for the estimated thermal properties $\hat{K}_0$, $\hat{K}_3$, $\hat{C}_0$, and $\hat{C}_3$, by assuming independent, constant variance errors, even though the errors can be correlated.

The variance–covariance matrix of the estimated thermal property vector $\hat{\mathbf{P}}$ is defined as:[20]

$$\text{var–cov}(\hat{\mathbf{P}})\equiv E\{[\hat{\mathbf{P}}-E(\hat{\mathbf{P}})][\hat{\mathbf{P}}-E(\hat{\mathbf{P}})]^{\mathrm{T}}\} \tag{14}$$

where $\hat{\mathbf{P}}\equiv\hat{\mathbf{P}}(\tilde{\mathbf{T}})$ is the unknown coefficient vector, $\tilde{\mathbf{T}}(x,t)$ is the measured interior temperature, $E(\bullet)$ denotes the statistical expected value (averaging) operator, and the superscript T refers to the transpose. Equation 14 is a nonlinear system for determining the variance–covariance matrix. In order to express it in the explicit conventional form shown in Equation 19, we linearize the right-hand side of Equation 14 by expanding $\hat{\mathbf{P}}$ and $E(\hat{\mathbf{P}})$ in a Taylor series and neglecting the higher order terms. We obtain

$$\text{var–cov}(\hat{\mathbf{P}})=\left[\frac{\partial\hat{\mathbf{P}}}{\partial\tilde{\mathbf{T}}^{\mathrm{T}}}\right]E\{[\tilde{\mathbf{T}}-E(\tilde{\mathbf{T}})][\tilde{\mathbf{T}}-E(\tilde{\mathbf{T}})]^{\mathrm{T}}\}\left[\frac{\partial\hat{\mathbf{P}}^{\mathrm{T}}}{\partial\tilde{\mathbf{T}}}\right] \tag{15}$$

For independent temperature measurements with constant variance, σ^2, we have[20]

$$E\{[\tilde{\mathbf{T}}-E(\tilde{\mathbf{T}})][\tilde{\mathbf{T}}-E(\tilde{\mathbf{T}})]^{\mathrm{T}}\}=\sigma^2\mathbf{I} \tag{16}$$

where $\mathbf{I}$ is the identity matrix. Introducing Equation 16 into Equation 15, results in the variance–covariance matrix:

$$\text{var–cov}(\hat{\mathbf{P}})=\sigma^2\left[\frac{\partial\hat{\mathbf{P}}}{\partial\tilde{\mathbf{T}}^{\mathrm{T}}}\right]\left[\frac{\partial\hat{\mathbf{P}}^{\mathrm{T}}}{\partial\tilde{\mathbf{T}}}\right] \tag{17}$$

The right-hand side of Equation 17 is written in inverse form as

$$\text{var–cov}(\hat{\mathbf{P}})=\sigma^2\left\{\left[\frac{\partial\tilde{\mathbf{T}}^{\mathrm{T}}}{\partial\hat{\mathbf{P}}}\right]\left[\frac{\partial\tilde{\mathbf{T}}}{\partial\hat{\mathbf{P}}^{\mathrm{T}}}\right]\right\}^{-1} \tag{18}$$

Here the Jacobian matrix $(\partial\tilde{\mathbf{T}}/\partial\hat{\mathbf{P}}^{\mathrm{T}})$ and its transpose $(\partial\tilde{\mathbf{T}}^{\mathrm{T}}/\partial\hat{\mathbf{P}})$ are evaluated from the results obtained by the finite difference solution of the problem.

The variance–covariance matrix can be written in explicit form as[20]

$$\text{var–cov}(\hat{\mathbf{P}})=\begin{bmatrix}\sigma^2_{\hat{K}_0} & \sigma_{\hat{K}_0\hat{K}_3} & \sigma_{\hat{K}_0\hat{C}_0} & \sigma_{\hat{K}_0\hat{C}_3}\\ \sigma_{\hat{K}_3\hat{K}_0} & \sigma^2_{\hat{K}_3} & \sigma_{\hat{K}_3\hat{C}_0} & \sigma_{\hat{K}_3\hat{C}_3}\\ \sigma_{\hat{C}_0\hat{K}_0} & \sigma_{\hat{C}_0\hat{K}_3} & \sigma^2_{\hat{C}_0} & \sigma_{\hat{C}_0\hat{C}_3}\\ \sigma_{\hat{C}_3\hat{K}_0} & \sigma_{\hat{C}_3\hat{K}_3} & \sigma_{\hat{C}_3\hat{C}_0} & \sigma^2_{\hat{C}_3}\end{bmatrix} \tag{19}$$

If we assume additive, independent errors, the nondiagonal elements in Equation 19 vanish. Then, a comparison of Equations 18 and 19 gives the standard deviation of the estimated properties, $\sigma_{\hat{\mathbf{P}}}$, as

$$\sigma_{\hat{\mathbf{P}}}=\sigma\sqrt{\text{diag}\left\{\left[\frac{\partial\tilde{\mathbf{T}}^{\mathrm{T}}}{\partial\hat{\mathbf{P}}}\right]\left[\frac{\partial\tilde{\mathbf{T}}}{\partial\hat{\mathbf{P}}^{\mathrm{T}}}\right]\right\}^{-1}} \tag{20}$$

where σ is the standard deviation of the measurements.

If we now assume a normal distribution for measurement errors, the 99% confidence bounds for the computed thermal property values, $\hat{P}_j$, is determined as[18]

$$\text{Probability}(\hat{P}_j-2.576\sigma_{\hat{P}_j}<\hat{P}_{j,\text{mean}}<\hat{P}_j+2.576\sigma_{\hat{P}_j})\cong 99\% \tag{21}$$

If we neglect the deterministic error (i.e., the error between the mean estimated value of the thermal property without the stochastic error and its own true value), Equation 21 becomes

$$\text{Probability}(\hat{P}_j-2.576\sigma_{\hat{P}_j}<\hat{P}_j<\hat{P}_j+2.576\sigma_{\hat{P}_j})\cong 99\% \tag{22}$$

Equation 22 defines the approximate statistical confidence bounds for the estimated property values; that is, we expect the estimated values of the parameters to lie between these two bounds, with a 99% confidence level.

Table 1 Data for estimated thermal properties for iron from exact and simulated inexact measurements

	Simulated normally distributed errors $\sigma=0.0$	$\sigma=0.01$	$\sigma=0.1$
K_0 (exact) $W m^{-1}$-C^{-1}	50.000	50.000	50.000
First estimates* of $\hat{K}_0$	53.872	53.904	54.208
$\hat{K}_0$ (final values)	50.000	50.036	50.368
% error	0.000%	0.072%	0.736%
$\mp 2.576\sigma_{\hat{K}_0}$	∓0.000	∓0.198	∓1.989
K_3 (exact) $W m^{-1}$-C^{-1}	59.000	59.000	59.000
First estimates* of $\hat{K}_3$	53.537	53.952	57.787
$\hat{K}_3$ (final values)	59.000	58.874	57.738
% error	0.000%	0.214%	2.140%
$\mp 2.576\sigma_{\hat{K}_3}$	∓0.000	∓0.492	∓4.877
C_0 (exact) $kJ m^{-3}$-C^{-1}	3600.0	3600.0	3600.0
First estimates* of $\hat{C}_0$	3651.8	3653.2	3662.5
$\hat{C}_0$ (final values)	3600.0	3604.3	3643.1
% error	0.000%	0.119%	1.197%
$\mp 2.576\sigma_{\hat{C}_0}$	∓0.000	∓23.64	∓236.2
C_3 (exact) $kJ m^{-3}$-C^{-1}	4500.0	4500.0	4500.0
First estimates* of $\hat{C}_3$	4306.9	4305.7	4297.0
$\hat{C}_3$ (final values)	4500.0	4495.2	4451.6
% error	0.000%	0.107%	1.076%
$\mp 2.576\sigma_{\hat{C}_3}$	∓0.000	∓25.00	∓249.8

* First estimates obtained from the solution of Equations 10 and 11.

Results

We first examine the accuracy of the inverse analysis by using the simulated exact results obtained from the direct solution of the problem as the measured temperature data taken at two interior thermocouples. To study the effect of measurement errors on the unknown property coefficients K_0, K_3, C_0, and C_3, we simulate the measure temperature containing measurement errors as follows:

$$T_{\text{measured}} = T_{\text{exact}} + \alpha\sigma \tag{23}$$

where σ is the standard deviation of measurement errors. For normally distributed errors with 99% confidence bounds, α lies within the bounds: $-2.576<\alpha<2.576$. The values of α are calculated randomly by the IMSL subroutine DRNNOR.[19]

We then use the measured temperature data simulated by Equation 23 to estimate the unknown property coefficients K_0, K_3, C_0, and C_3 from the solution of Equations 10 and 11. In order to solve Equations 10 and 11, we need to choose at least two different values of t_j. Solving these equations with different t_j values has shown that the property coefficients are not very sensitive to t_j values. We then use the results obtained from Equations 10 and 11 as first estimates in the least squares equation, Equation 12, and continue iterations until we satisfy a specified convergence criterion.

Numerical experimentation

We ran several test cases on a computer to determine the accuracy of the inverse analysis. We let the specimen thickness be $L=0.03$ m, the total temperature measuring time be 300 s, and the measurement-time step be 20 s, which corresponds to 15 temperature readings per thermocouple. We used two different heat input data in the calculation: $q=25{,}000\, W m^{-2}$ for iron and $q=100\, W m^{-2}$ for fiberglass. Thermal property coefficients were $K_0=50\, W m^{-1}$-C^{-1}, $K_3=59\, W m^{-1}$-C^{-1}, $C_0=3{,}600\, kJ m^{-3}$-C^{-1}, and $C_3=4{,}500\, kJ m^{-3}$-C^{21} for iron and $K_0= 0.04\, W m^{-1}$-C^{-1}, $K_3=0.07\, W m^{-1}$-C^{-1}, $C_0=13\, kJ m^{-3}$-C, and $C_3=14\, kJ m^{-3}$-C^{21} for fiberglass. Such a selection covers a sufficiently broad range for the property variation.

We now consider typical simulated applications to illustrate the effectiveness of the inverse solution. First, we computed the estimated property coefficients by using the exact temperature data. Then, we introduced measurement errors into the exact temperatures to simulate the measured temperatures and the calculated properties. The results of these calculations are presented in Table 1 for the case of iron and in Table 2 for the case of fiberglass as the sample materials. In Tables 1 and 2, the first estimates for the property coefficients are from the solution of Equations 10 and 11. We used three different standard deviations for measurement error: $\sigma=0$ (exact), $\sigma=0.01$, and $\sigma=0.1$. Clearly, the exact input data produce exact results for the estimated properties K_0, K_3, C_0, and C_3, which means zero deterministic error. As expected, the error in the estimated thermal properties increases as the standard deviation for the measurement temperature increases from $\sigma=0.01$ to $\sigma=0.1$ for both cases.

We calculated the 99% confidence bounds for the estimated properties by using the estimated property data obtained from Tables 1 and 2 and utilizing Equation 22. The results are presented in Figures 3 and 4 for iron and fiberglass, respectively, and for standard deviations of $\sigma=0.01$ and $\sigma=0.1$. Figures 3 and 4 show that the 99% confidence bounds increase with increasing distance from the heated surface, which implies that the estimated results become more sensitive to measurement errors with increasing distance from the heated surface. Note that the confidence bounds for fiberglass are narrower than for iron. The reason is that the property gradient with respect to temperature, i.e., $\partial\hat{\mathbf{P}}/\partial\hat{\mathbf{T}}^T$, for fiberglass (on the right-hand side of Equation 17) is smaller than that for iron, because temperature variation affects the thermal diffusivity of iron more than that of fiberglass. Furthermore, thermal conductivity varies with temperature more than heat capacity does. Thus the change in confidence bounds with distance for thermal conductivity is more than that for heat capacity.

Conclusions

A new expression is developed for making sufficiently accurate initial guesses to start the iterations in the inverse problem for

Table 2 Data for estimated thermal properties for fiberglass from exact and simulated inexact measurements

	Simulated normally distributed errors $\sigma=0.0$	$\sigma=0.01$	$\sigma=0.1$
K_0 (exact) $W m^{-1}$-C^{-1}	0.0400	0.0400	0.0400
First estimates* of $\hat{K}_0$	0.0421	0.0421	0.0421
$\hat{K}_0$ (final values)	0.0400	0.0400	0.0401
% error	0.000%	0.023%	0.250%
$\mp 2.576\sigma_{\hat{K}_0}$	∓0.000	0.000051	∓0.000512
K_3 (exact) $W m^{-1}$-C^{-1}	0.0700	0.0700	0.0700
First estimates* of $\hat{K}_3$	0.0674	0.0676	0.0689
$\hat{K}_3$ (final values)	0.0700	0.0699	0.0695
% error	0.000%	0.143%	0.714%
$\mp 2.576\sigma_{\hat{K}_3}$	∓0.000	∓0.000156	∓0.001552
C_0 (exact) $kJ m^{-3}$-C^{-1}	13.000	13.000	13.000
First estimates* of $\hat{C}_0$	12.957	12.957	12.961
$\hat{C}_0$ (final values)	13.000	13.004	13.048
% error	0.000%	0.030%	0.372%
$\mp 2.576\sigma_{\hat{C}_0}$	∓0.000	∓0.020322	∓0.203172
C_3 (exact) $kJ m^{-3}$-C^{-1}	14.000	14.000	14.000
First estimates* of $\hat{C}_3$	13.851	13.850	13.840
$\hat{C}_3$ (final values)	14.000	13.993	13.932
% error	0.000%	0.050%	0.486%
$\mp 2.576\sigma_{\hat{C}_3}$	∓0.000	∓0.024397	∓0.243907

* First estimates obtained from the solution of Equations 10 and 11.

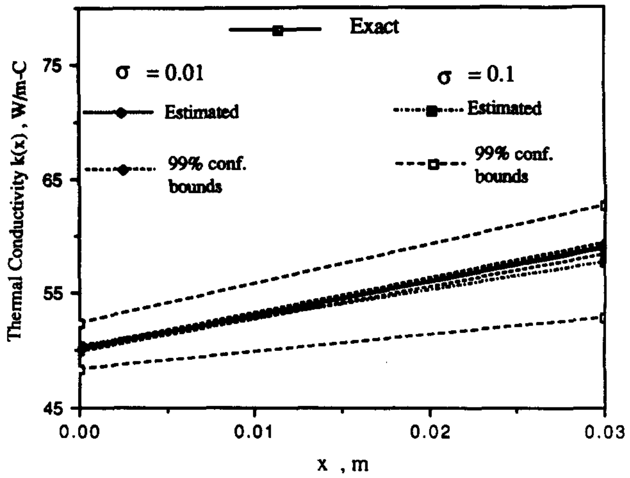

Figure 3(a) Effects of σ on the estimation of thermal conductivity for iron by inverse analysis

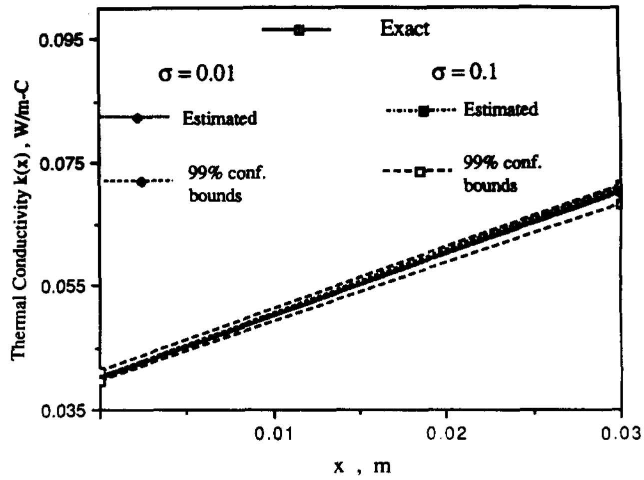

Figure 4(a) Effects of σ on the estimation of thermal conductivity for fiberglass by inverse analysis

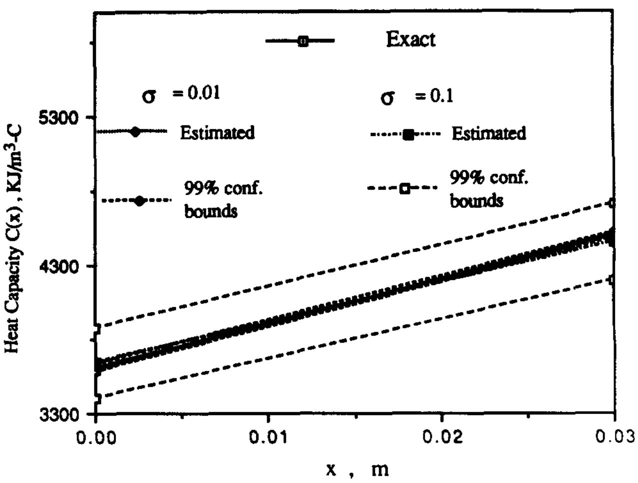

Figure 3(b) Effects of σ on the estimation of heat capacity for iron by inverse analysis

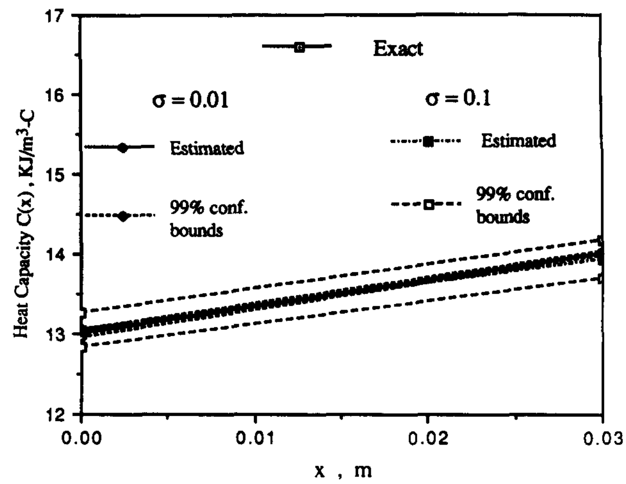

Figure 4(b) Effects of σ on the estimation of heat capacity for fiberglass by inverse analysis

simultaneously estimating spatially varying thermal conductivity and heat capacity per unit volumes. Once the initial estimates are available, the Levenberg–Marquardt method is applied to refine the results to within a specified convergence criterion. A statistical analysis is utilized to develop confidence bounds; the estimated values of the coefficients lie within these confidence limits.

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