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A Hybrid Algorithm for Simultaneous Retrieval of Thermal Conductivity and Time-Dependent Heat Flux

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Abstract: This paper presents a hybrid technique for simultaneous estimation of parameter and function in inverse heat conduction problems. No prior information is used for the functional form of the heat flux in the present study. The scheme presented here is a combination of two different classical methods: The Variable Metric Method (VMM) and Gauss Method (GM). The determination of the unknown thermal coefficients includes two steps per iteration of the estimation algorithm: the function estimation step; and the parameter estimation step. VMM and GM are used to handle function estimation and parameter estimation problems, respectively. It is shown via simulated experiment that unknown quantities can be obtained with reasonable accuracy using this method despite existing noise in the measurement data.

Keywords: Gauss Method, Index Terms-Function Estimation, Inverse Problems, Parameter Estimation, Variable Metric Method.

1. Introduction

The prediction of thermal coefficients in a thermal system has many engineering applications in various branches of science and engineering. This can be achieved via providing information in other parts of the system through special equipments. Such problems involve a variety of challenges and have received considerable attention from many researchers in recent years [1]. Assessment of boundary conditions or of the thermophysical properties of a conductive body from the measurements of temperature at a few points in the domain is typically called the inverse heat conduction problem (IHCP). This happens when the direct measurement of those quantities is unfeasible. The solution of inverse problems is not straightforward as the unavoidable noise in the data can produce large or even unbounded deviations in the results. This is due to “ill posed” nature of the IHCP [1-7]. In general, solution of the IHCP can be achieved via minimization of a sum of squared error function; which is focused on the difference between the values of the measured temperatures and those obtained by an efficient computational method. The unknown thermal coefficients on the mathematical model (i.e., thermal properties, boundary or initial conditions) that lead to an acceptable value for the aforementioned error function (for example based on the iterative regularization method) are the solution of the IHCP [8-15].

IHCPs are usually categorized as parameter and function estimation problems. The parameter estimation problems show the identification of a relatively small number of unknowns; the parameters are often coefficients in the governing equations. Examples of these parameters are thermal conductivity, thermal emittance, convection coefficient, specific heat, density, and even the parameters that appear in the studies of turbulent flows. Many researchers have employed different inverse methods to determine unknown parameters [12-16]. On the other hand, a function estimation problem determines functions represented by numerous unknowns, which may vary spatially and temporally. Function estimation problems have been the subject of extensive investigations, thanks to their numerous and various applications [1,11]. It is worth mentioning that an IHCP may be a combined parameter and function estimation problem. Anillustration can be found in the simultaneous prediction of heat flux and thermal

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conductivity of a heat-conducting body, which is exposed to an unknown heat flux. Assessment of thermophysical properties utilizing experimental techniques not only demands the knowledge of recorded temperature history during the test, but also the transient heat flux profile should be valid. Paradoxically, the bibliography on combined parameter and function estimation in the fundamental equation of the heat transfers is very limited; Loulou and Artioukhine discussed the application of numerical algorithms based on gradient-type methods for recovering unknown variables. As the descent variable in gradient-type methods is chosen to be the same for the independent unknowns, the very slow or no convergence at all of the gradient-type methods can be observed. To overcome this difficulty, Loulou and Artioukhine presented a discussion of the implementation of the iterative algorithms for solving the general problem of recovering a complete set of thermal coefficients; and introduced a vectorial descent variable and reported a considerable increase in the convergence rate [17].

The purpose of this research is to develop an efficient and uncomplicated method for simultaneously predicting the unknown parameters and functions in an IHCP. The method is quite different from the previous method of Loulou and Artioukhine [17]. On the basis of the proposed approach, the determination of the unknown thermal coefficients includes two steps per iteration of the estimation algorithm: The function estimation step; and the parameter estimation step. A flowchart showing the sequence of calculations in the algorithm is given in Fig. 1. After initial setting of the unknown parameters and function, the solver repeatedly cycles through the following steps:

1- In the function estimation process, by using initial guess values for the unknown thermal conductivity, the IHCP becomes a function estimation problem. Estimated function (heat flux) by using Variable Metric Method with Adjoint Problem (VMMAP) is then used for parameter estimation procedure.

2- In this procedure, the parameters will denote as the unknown variables and will recover using Gauss Method (GM) based on the knowledge of function estimated at the previous step. It should be noted that this procedure repeats for each unknown parameter.

3- Then an intermediate set of the thermal coefficient values is substituted for the unknown parameters and function in the following analysis. Several iterations are needed before obtaining the undetermined thermal coefficients.

2. Direct problem

The physical problem considered in this article consists of a one-dimensional slab of thickness L initially at the temperature $T_0(x)$. The surface of the slab at x = L is heated with a heat flux q(t), while the other surface at x = 0 is kept insulated. The mathematical formulation for the physical problem considered here can be written as:

$$\rho C_p \frac{\partial T}{\partial t} = k \frac{\partial^2 T}{\partial x^2} \qquad 0 \le x \le L \tag{1}$$

$$-k \frac{\partial T}{\partial x} = q(t) \qquad x = L \tag{2}$$

$$\frac{\partial T}{\partial x} = 0 \qquad x = 0 \tag{3}$$

$$T(x,0) = T_0 \qquad 0 \le x \le L \tag{4}$$

3. Inverse problem formulation

In the inverse problem considered in this study, the time-dependent heat flux and thermal conductivity are regarded as being unknowns and to be estimated from measured temperatures by sensors. These unknown variables are gathered in a single unknown vector $\vec{P} = \left[q(t), k \right]$. The solution of present inverse problem is to be sought in such a way that the following functional is minimized:

$$S\left(\vec{P}\right) = \sum_{i=1}^{N} \sum_{j=1}^{M} \left(Y_{i,j} - T_{i,j}\left(\vec{P}\right) \right)^2 \tag{5}$$

where $Y_{i,j}$'s are the measured temperatures and $T_{i,j}$'s are the estimated temperatures at the measurement locations obtained by the developed direct code. M is the number of total time steps, and iN is the number of the used sensors. As the problem is simultaneously of parameter and function estimation type, a combined procedure is proposed to handle it. This procedure is based on two different methods: VMMAP for the function estimation stage (i.e., heat flux); and GM for the parameter estimation stage.

3.1. Function estimation stage

In the function estimation stage, initial value is assumed for the thermal conductivity (i.e., the initial guess values, which are improved during the iterative

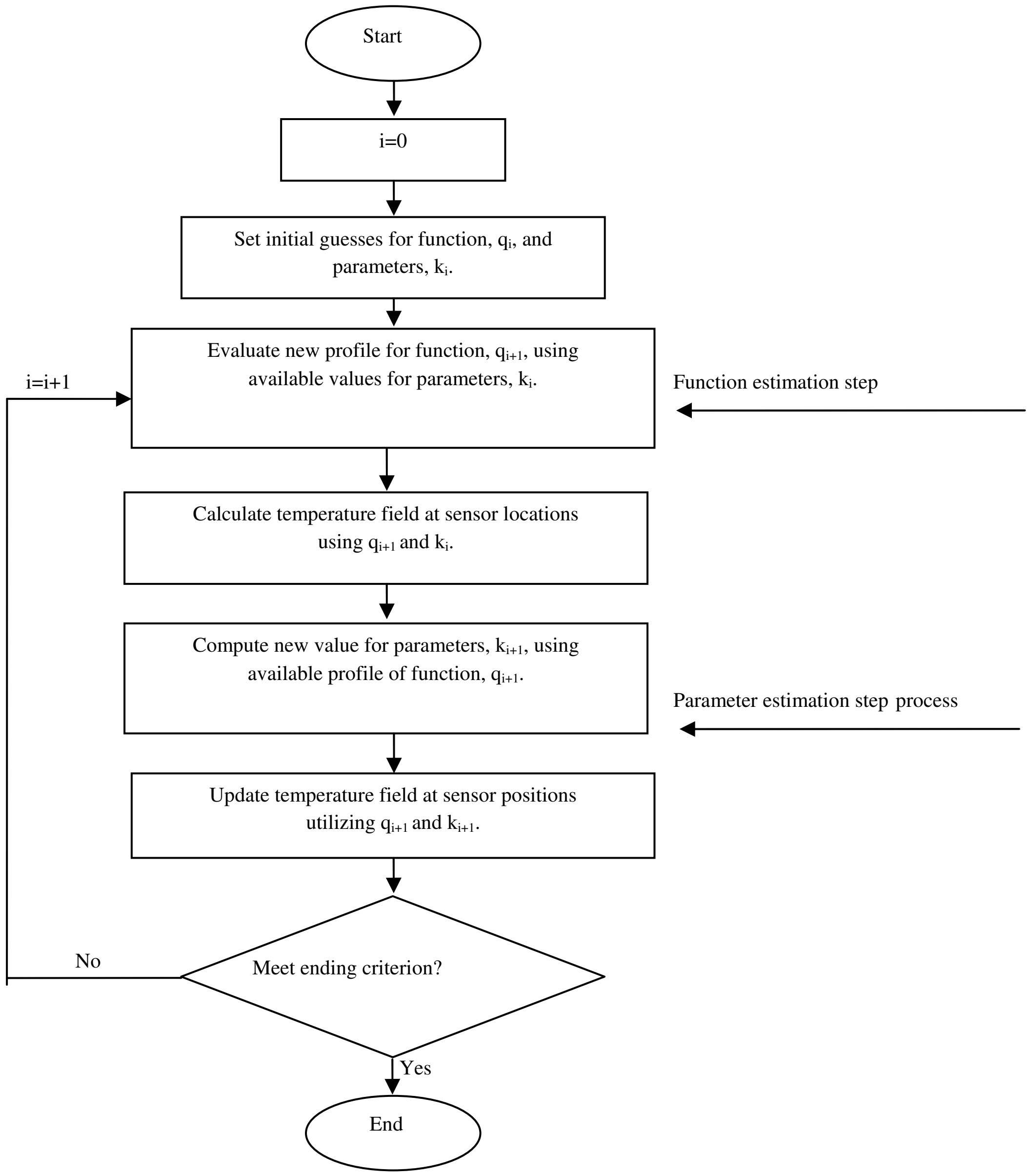

Fig. 1. A flowchart of the combined parameter and function estimation strategy

process) and then the unknown function (i.e., heat flux) can be estimated by using temperature measurements taken within the slab. The components of heat flux function are determined via minimization of the following functional:

$$J\left[q(t)\right]=\sum_{j=1}^{N}\int_{t=0}^{t_f}\left\{Y_j(t)-T\left[x_j,t;q(t)\right]\right\}^2 dt \tag{6}$$

Among the well-known methods for boundary estimation problems, the gradient methods have received the most attention. The minimization procedure of the function (6) by utilizing the gradient-type methods is built as follows:

$$q_{i+1}(t)=q_i(t)-\beta_i d_i(t) \tag{7}$$

where the superscript i is the iteration number, β_i is the optimal step length and $d_i(t)$ is search direction. The success of these methods depends on effective choices of both the direction $d_i(t)$ and the step length β_i. Depending on the selection of search direction, various types of gradient methods exist. The search direction often has the form:

$$d_i(t)=-B_i^{-1}\nabla f_i \tag{8}$$

In the steepest descent method B_i is simply the identity matrix, while in Newton's method B_i is the exact Hessian $\nabla^2 f_i$. In the Fletcher–Reeves form of the conjugate gradient method, $(B_i)^{-1}$ has the following form [18]:

$$(B_{i+1})^{-1} = \left(I - \frac{d_i \nabla f_{i+1}^{\ T}}{\nabla f_i^{\ T} \nabla f_i} \right) \tag{9}$$

where $s_i = \beta_i d_i(t)$. In quasi-Newton methods, B_i is an approximation to the Hessian that is updated at every iteration by means of a low-rank formula. For instance, the BFGS version of VMM uses the following equation for $(B_i)^{-1}$[18]:

$$(B_{i+1})^{-1} = \left(\frac{S_i S_i^T}{[\nabla f_i - \nabla f_i]^T S_i} \right) + \left(I - \frac{S_i [\nabla f_{i+1} - \nabla f_i]^T}{[\nabla f_{i+1} - \nabla f_i]^T S_i} \right) (B_i)^{-1} \left(I - \frac{S_i [\nabla f_{i+1} - \nabla f_i] S_i^T}{[\nabla f_{i+1} - \nabla f_i]^T S_i} \right) \tag{10}$$

As mentioned in [10], the accuracy of four versions of VMM does not differ appreciably from each other. Then, there is no attempt made here to consider the behavior of four available versions of the VMMAP and the interested reader is referred to [10,18] for a more detailed discussion.

The optimal step length β_i is chosen as the one that minimizes the function f[q(t)] at each iteration i. By using a first-order Taylor series approximation and performing the minimization, the following expression results for the search step size:

$$\beta_i = \frac{\int_{t=0}^{t_f} \{ T[x_j, t : q(t)] - Y_j(t) \} \Delta T[x_j, t : d_i(t)] dt}{\int_{t=0}^{t_f} \{ \Delta T[x_j, t : d_i(t)] \}^2 dt} \tag{11}$$

For the implementation of the iterative procedure described here the sensitivity term $\Delta T[x_j, t : d_i(t)]$ and gradient $\nabla f[q_i(t)]$ are required. The former is determined with the sensitivity problem and the latter with adjoint problem. Both problems are briefly described next.

a. The sensitivity problem

The sensitivity problem is used to determine the variation of the dependent variables due to the changes in the unknown quantity. Therefore, the sensitivity problem can be obtained by assuming that the temperature T(x,t) is perturbed by an amount ΔT(x,t), when the unknown heat flux q(t) is perturbed by Δq(t) in the specific direction. Thus, the following problem for the sensitivity function ΔT(x,t) can be obtained:

$$\rho C_P \frac{\partial (\Delta T)}{\partial t} = k \frac{\partial^2 (\Delta T)}{\partial x^2} \qquad 0 \le x \le L \tag{12}$$

$$-k \frac{\partial \Delta T}{\partial x} = \Delta q(t) \qquad x = L \tag{13}$$

$$\frac{\partial \Delta T}{\partial x} = 0 \qquad x = 0 \tag{14}$$

$$\Delta T(x,0) = 0 \qquad 0 \le x \le L \tag{15}$$

b. The adjoint problem

In order to derive the adjoint problem for heat flux, (1) is multiplied by the Lagrange multiplier function λ(x,t), and the resulting expressions are integrated over the time and the space domain. Then the final results are added to the right hand side of (6) to yield the following expression for the functional f [q(t)]:

$$J[q(t)] = \int_{t=o}^{tf} \{ Y_j(t) - T[L,t:q(t)] \}^2 dt + \int_{t=0}^{tf} \int_{x=0}^{L} \lambda(x,t) \left(k \frac{\partial^2 T}{\partial x^2} - \rho C_p(t) \frac{\partial T}{\partial t} \right) dx\, dt \tag{16}$$

The variation Δf is obtained by perturbing q by Δq and T by ΔT in (16), subtracting from the resulting expression the original (16) and neglecting the second-order terms. We thus find:

$$\Delta J[q(t)] = \int_{t=0}^{tf} \int_{x=0}^{L} \lambda(x,t) \left(k \frac{\partial^2 \Delta T}{\partial x^2} - \rho C_p(t) \frac{\partial \Delta T}{\partial t} \right) dx\, dt + 2 \int_{t=0}^{tf} \{ Y_j(t) - T[L,t:q(t)] \} \delta(x_j - x_s) \Delta T\, dt \tag{17}$$

Using integration by parts as well as the boundary and initial conditions, the derivatives are transferred to the lagrange multiplier function. After some algebraic manipulation, the following adjoint differential equation is obtained for the lagrange multiplier function λ(x,t)

$$\rho C_p \frac{\partial \lambda}{\partial t} = k \frac{\partial^2 \lambda}{\partial x^2} \qquad 0 \le x \le L \tag{18}$$

$$-k \frac{\partial \lambda}{\partial x} = 2(T - Y) \qquad x = L \tag{19}$$

$$\frac{\partial \lambda}{\partial x} = 0 \qquad x = 0 \tag{20}$$

$$\lambda(x, t_f) = 0 \qquad 0 \le x \le L \tag{21}$$

When λ (x,t) satisfies the above differential equation, the functional given by (17) reduces to:

$$\Delta J\left[q(t)\right] = -\int_{t=0}^{t_f} \Delta q(t)\lambda\,(L,t)dt \tag{22}$$

By definition, the functional increment can be presented as:

$$\Delta J\left[q(t)\right] = \int_{t=0}^{t_f} \Delta q(t)\nabla J\left[q(t)\right]dt \tag{23}$$

A comparison of (22) and (23) leads to the following expression for the gradient of functional

$$\nabla J\left[q(t)\right] = -\lambda(L,t) \tag{24}$$

3.2. Parameter estimation stage

In the parameter estimation stage, the thermal conductivity denotes as the unknown variable and recover based on the knowledge about the estimated function at the previous stage. The solution to the present inverse problem can be determined by satisfying the following equation:

$$F(k) = \sum_{j=1}^{N}\int_{t=0}^{t_f}\left\{Y_j(t) - T\left[x_j,t;k\right]\right\}^2 dt \tag{25}$$

One of the prevalent iterative methods for minimizing the objective function, F, is the GM. The computational procedure for the estimation of the unknown parameters at iteration i can be summarized as follows:

1- Solve the direct problem with available estimated k_i in order to obtain temperature field within the slab $T(k_i)$.

2- Compute F from the (25).

3- Compute the sensitivity matrix X defined by the following equation:

$$X = \left[\frac{\partial T_{1,1}}{\partial k} \quad \frac{\partial T_{1,2}}{\partial k} \quad . \quad .\frac{\partial T_{N,M}}{\partial k}\right]^T \tag{26}$$

4- Solve the following linear system of equation to find Δk_i.

$$\left[X^T{}_i X_i\right]\Delta k_i = X^T{}_i\left(\vec{T}_i - \vec{Y}_i\right) \tag{27}$$

where superscript T denotes transpose sign, and vectors $\vec{T}$ and $\vec{Y}$ are defined as:

$$\vec{T}_i = \left[T_{1,1}, T_{1,2}, ..., T_{1,M}, T_{2,1}, T_{2,2}, ...T_{2,M}, ..., T_{N,M}\right]_i \tag{28}$$

$$\vec{Y}_i = \left[Y_{1,1}, Y_{1,2}, ..., Y_{1,M}, Y_{2,1}, Y_{2,2}, ..., Y_{2,M}, ..., Y_{N,M}\right]_i \tag{29}$$

5- The updating rule for the BKM's algorithm is then applied to determine the unknown parameter

$$k_{i+1} = k_i + \Delta k_i \tag{30}$$

6- Solve the direct problem with this new estimated k_{i+1} in order to obtain $T(k_{i+1})$; and then compute F, as defined by (25).

7- Check the stopping (convergence) criterion given by (31):

$$F\left(k_{i+1}\right) < \varepsilon \tag{31}$$

8- Stop the iteration procedure if (31) is satisfied; otherwise, replace i by i+1 and return to step 3.

3.3. Computational procedure for inverse methodology

The computational procedure for the estimation of the unknown parameters can be summarized as follows:

1- Choose initial guess q_0 and k_0.

2- Solve the direct problem with q_i and k_i to obtain temperature at sensor locations.

3- Evaluate the objective functional, S, using (5).

4- Calculate heat flux, q_{i+1}, as described in the function estimation stage.

5- Solve the direct problem with estimated heat flux at previous stage, q_{i+1}, in order to obtain temperatures at sensor locations.

6- The updating rule for the GM's algorithm is then applied to determine the unknown parameters, k_{i+1}. This procedure applies individually for each parameter.

7- Check the stopping criterion given by (32):

$$S\left(\vec{P}^{(i+1)}\right) < \varepsilon \tag{32}$$

where ε is a small number (O(10^{-4} ~ 10^{-6})). However, in the presence of unavoidable noise embedded in the data, the iterative process is stopped according to the discrepancy principle criterion [19], i.e., upon satisfaction of the following condition:

$$S\left(\vec{P}\right) = \sum_{i=1}^{N}\sum_{j=1}^{M}\left[Y_{i,j} - T_{i,j}\left(\vec{S}\right)\right]^2 \approx \sum_{i=1}^{N}\sum_{j=1}^{M}\sigma_{i,j}{}^2 \approx \delta \tag{33}$$

where δ is the integrated error of the measured data at time t_j and having $\sigma_{i,j}$ as standard deviation. If the standard deviation is adopted to be the identical for all data measurements, then the compacted error will have the following statement:

$$\delta = N \times M \times \sigma^2 \tag{34}$$

where σ is the standard deviation of the errors in the temperature. The discrepancy principle is based on terminating the procedure as soon as the objective functional is in the order of magnitude of the compacted error, which represents the best evaluation expected in the order of the data error.

4. Results and discussions

In order to demonstrate the accuracy and efficiency of the present method, a simulated test case for simultaneous parameter and function estimation is considered. Following values are used for the materials properties, boundary and initial conditions in this test case: k=75 (W/m.K), ρCp=3729 (kJ/m^3.K), L=5 cm, T_0=300 K and the heat flux function, q(t), is assumed to have rectangular (or pulsed) form. The duration of the experiment was assumed to be 100 s. A computational grid with 51 spatial nodes is used to solve the problem. The number of time-steps taken is 101. The measured temperature on the exposed surface, Y(t), applied in the function estimation procedure are obtained from numerical simulations by the developed numerical code. These data are perturbed by adding random errors to their exact values, Y_{exact}(t).

$$Y(t) = Y_{exact}(t) + \omega\sigma \tag{35}$$

where ω is a random variable being within -2.576 to 2.576 for a 99% confidence bound and variable σ is the standard deviation. Two sensors are assumed to be located at x = 0 (cm) and x = 4 (cm). The temperature values were obtained using the direct heat conduction calculations and their values at sensor locations are saved and used as sensors data.

In order to specify the deviation of the estimated thermal coefficients ($\hat{q}(t)$ and $\hat{k}$) from the exact ones ($q(t)$ and k), relative errors are defined as follows:

$$q_{error} = \frac{\int_{t=0}^{t_f} \left[q(t_i) - \hat{q}(t_i) \right]^2 dt}{\int_{t=0}^{t_f} \left[q(t_i) \right]^2 dt} \times 100\% \tag{36}$$

$$k_{err} = \left| \frac{k - \hat{k}}{k} \right| \times 100\% \tag{37}$$

The initial guess values for q(t) and k in the current algorithm are taken to be 1000 (W/m^2) and 5 (W/m.K), respectively. The results obtained using exact and inexact data and two stopping criteria are summarized in table 1. Using errorless data, the excellent agreement between the exact solutions and the estimated results can be seen. In this situation, heat flux and thermal conductivity are recovered their theoretical values and the corresponding relative error is machine zero. The close agreement between the exact solutions and the estimated values underlines the capability of the algorithm to finding the accurate values in IHCP.

It was observed that the difference between the values of the predicted heat flux and the exact solution is indistinguishable, even at the areas of rapid increases/decreases in the heat flux (at the elapsed times of 20 and 80 s). Due to using the exact measurements, the desired stopping criterion in this case is given by (32) and the precision is taken to be $\varepsilon = 10^{-6}$.

At the next stage, the verification of the proposed strategy for solving the IHCP with noisy data is considered. The measured temperatures with $\sigma = 5$ are obtained according to (35). The stopping criterion in this case is based on the discrepancy principle, (33). Fig. 2 demonstrates the retrieved heat flux. As expected, the largest errors appear near the sharp discontinuities. It is observed that the error of the estimated function is small in comparison to the added noise and reliable results can still be obtained when measurement errors are included. The reduction of the objective functional for two sets of data is plotted in Fig. 3. As can be seen, using noise-free data, the objective function leads to significantly smaller values for the objective function noisy data.

Table 1. Results of estimating heat flux

Data	Heat Flux		Thermal Conductivity	
	Initial Guess	q_{err} %	Estimated value	k_{err} %
Noise-free	1000	3×10^{-10}	75.00002	2.5×10^{-5}
Noisy (σ=5)	1000	0.76	74.46	0.72

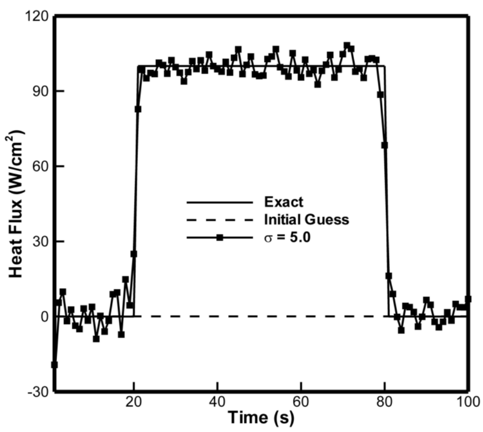

Fig. 2. The exact and estimated values of heat flux (noisy data)

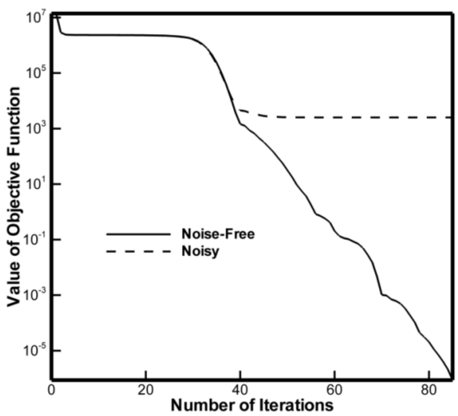

Fig. 3. Reduction histories of the objective function for errorless and noisy data

4. Conclusions

A framework is introduced for taking advantage of the traditional techniques in combined parameter and function estimation problems and broadening their appeal through a basic understanding of their application. To take into account the benefits of the variable metric method in handling function estimation problems as well as the Gauss method advantages in parameter estimation problems, a joint method for solving combined parameter and function estimation problems was used in this paper. In general, the numerical results showed that the proposed methodology in this study yields reliable estimation of the unknown thermal coefficients in the range of desired accuracy.

Nomenclature

C_P	specific heat, J/kg.K
d	descent direction
dl	time step, s
f	the objective functional
B	identity matrix (in the steepest descent method)
I	identity matrix
J	the objective functional for function estimation problem
K	thermal conductivity, W/m.K
k_i	unknown parameter
L	slab thickness, m
M	number of total time steps
N	number of sensors
P	vector of unknown parameters
q(t)	unknown surface heat flux, W/m^2
S	the objective functional for combi-ned parameter and function estimation problem
T	temperature, K
T_0	initial temperature, K
t	time, s
t_f	final time, s
Y	temperature measured by sensors, K
X	sensitivity matrix
x	space variable, m
β	the optimal step length
Δ	small variation
ΔT	sensitivity function
δ	integrated error
ε	very small value
λ	adjoint variable
ρ	density, kg/m^3
σ	standard deviation of the errors in the measured temperatures
ω	random variable
∇f	gradient of the objective functional

Subscripts

i	iteration number
j	iteration number
exact	exact value

Superscripts

T	transpose of a matrix
□	estimated value

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