Optimal regularization method to determine the strength of a plane surface heat source

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The regularization method combined with the generalized cross-validation (GCV) approach is used to solve the problem of inverse heat conduction involving the determination of the strength of a surface heat source located inside a plate. The advantage of the present approach lies in the fact that the GCV method allows the determination of the optimum value of the regularization parameter. Numerical experiments are presented to show that the value of the regularization, α, determined in this manner is indeed optimum.

Keywords: inverse conduction; internal heat source determination; optimal regularization; transient conduction

Introduction

The direct heat conduction problems are concerned with the determination of temperature at interior points of a region when the initial and boundary conditions and heat generation are specified. In contrast, the inverse heat conduction problem (IHCP) involves the determination of the surface conditions, energy generation, properties, etc., from the knowledge of the temperature measurements taken within the body.

Various approaches are available to solve the inverse problems,[1] and the regularization methods[2,3] appear to be very promising. In this approach, a proper regularization term needs to be added to the sum-of-squares error term in order to stabilize the solution. Presently there is no way to estimate the optimum value of the regularization parameter by using the measured data only. All the existing work on this subject requires that the noise level in the data should be known.[3–5] Because of this restriction, the available approaches are not practical.

The generalized cross-ventilation (GCV) method has been used in areas including smoothing noise data,[6] spline smoothing,[7] choosing a good ridge parameter,[8] and dynamic programming[9] to stabilize the solution. Recently the method had been tried in solving the inverse heat conduction problems[10–13] by the application of the dynamic programming approach.

In the present work, we apply the GCV method directly to the least squares equation approach for the solution of linear inverse heat conduction problems and show that the combined method is very fast and easy to apply for these solutions. Once the optimal value of regularization parameter is determined, the inverse solution process does not require iterations.

Problem formulation

A slab of unit thickness is initially at zero temperature. For time >0, a continuous plane surface heat source of unknown strength $G(t)$, located at specified position $x=0.5$, releases its energy continuously, while the boundary surfaces at $x=0.0$ and $x=1.0$ are both kept insulated (see Figure 1). The inverse analysis is concerned with the determination of the strength of this unknown energy source as a function of time from the transient temperature recording taken at the wall. The mathematical formulation of the problem is given by

$$\frac{\partial^2 T(x,t)}{\partial x^2}+\frac{1}{k}G(t)\,\delta(x-0.5)=\frac{1}{\lambda}\frac{\partial T(x,t)}{\partial t} \tag{1a}$$

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

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

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

where the thermal diffusivity, λ, and the thermal conductivity, k, are assumed to be constant, and the unknown plane surface heat source $G(t)$ is located at $x=0.5$. Here δ is the Dirac delta function and the source $G(t)$ varies continuously over time.

With one sensor placed at the boundary $x=1$, and temperature measurements taken at times t_j, $j=1,2,\ldots,M$, there is a total of M measurement data. The objective of this study is to determine the unknown strength of the source $G(t)$ by utilizing these M temperature data obtained at $x=1$.

Inverse solution by regularization method

The direct problem given by Equations 1 is solved by the Crank–Nicolson method. The regularization method used to solve the inverse problem is described below.

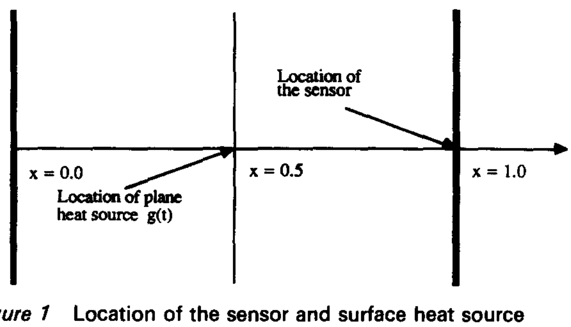

Figure 1 Location of the sensor and surface heat source

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The regularization method is a modification of the sum-of-squares function with the addition of the regularization terms. These additional terms have a smoothing effect on the internal heat source components by acting to minimize the effects of noise data.

Scott and Beck[14] have shown that as the order of regularization increases, the bias errors decrease and the variance increases. Thus the zero-order regularization has higher bias errors, while the second-order regularization is more sensitive to the random errors. Therefore as a compromise, the first-order regularization is chosen in this work.

The whole-domain first-order regularization procedure for a single sensor is given in matrix form as[1]

$$S=(\mathbf{Y}-\mathbf{T})^T(\mathbf{Y}-\mathbf{T})+\alpha(\mathbf{H}_1\mathbf{g})^T(\mathbf{H}_1\mathbf{g}) \tag{2}$$

where the scalar α is the regularization parameter, **Y** and **T** are the measured and estimated temperature vectors, respectively, **g** is the estimated heat source vector, and $\mathbf{H}_1$ is a square matrix associated with the first-order regularization procedures and is given by

$$\mathbf{H}_1=\begin{bmatrix} -1 & 1 & 0 & 0 & \dots & 0 \\ 0 & -1 & 1 & 0 & \dots & 0 \\ 0 & . & . & . & -1 & 1 \\ 0 & 0 & . & . & 0 & 0 \end{bmatrix}_{M\times M} \tag{3}$$

Later in the analysis we shall need $\mathbf{H}_1^T\mathbf{H}_1$, which is determined as

$$\mathbf{H}_1^T\mathbf{H}_1=\begin{bmatrix} 1 & -1 & 0 & 0 & 0 & \dots & \dots & 0 \\ -1 & 2 & -1 & 0 & 0 & \dots & \dots & 0 \\ 0 & -1 & 2 & -1 & 0 & \dots & \dots & 0 \\ 0 & . & . & . & . & -1 & 2 & -1 \\ 0 & 0 & . & . & . & . & -1 & 1 \end{bmatrix}_{M\times M} \tag{4}$$

Equation 2 is minimized with respect to **g** (where $\mathbf{g}=g_j$, $j=1,2,\dots,M$), and then rearranged in the form

$$\mathbf{X}^T(\mathbf{Y}-\mathbf{T})=\alpha\mathbf{H}_1^T\mathbf{H}_1\mathbf{g} \tag{5}$$

where **X** is the sensitivity coefficient matrix defined by

$$\mathbf{X}\equiv\partial\mathbf{T}/\partial\mathbf{g}^T \tag{6}$$

A Taylor series expansion of **T** with respect to an arbitrary value of the generation $\mathbf{g}_0$, gives

$$\mathbf{T}=\mathbf{T}_0+\frac{\partial\mathbf{T}}{\partial\mathbf{g}}(\mathbf{g}-\mathbf{g}_0) \tag{7}$$

where $\mathbf{T}_0$ is the value of temperature resulting from a generation $\mathbf{g}_0$. Therefore if we let $\mathbf{g}_0=0$, then $\mathbf{T}_0$ becomes $\mathbf{T}|_{\mathbf{g}=0}=0$. We now introduce these values of $\mathbf{g}_0=0$ and $\mathbf{T}_0=0$ into Equation 7 and the resulting expression into Equation 5 and solve for **g** to obtain

$$\mathbf{g}=[\mathbf{X}^T\mathbf{X}+\alpha\mathbf{H}_1^T\mathbf{H}_1]^{-1}\mathbf{X}^T\mathbf{Y} \tag{8}$$

The sensitivity coefficient matrix defined by Equation 6 can be expressed explicitly as

$$\mathbf{X}=\begin{bmatrix} \frac{\partial T_1}{\partial g_1} & \frac{\partial T_1}{\partial g_2} & \dots & \frac{\partial T_1}{\partial g_M} \\ \frac{\partial T_2}{\partial g_1} & \frac{\partial T_2}{\partial g_2} & \dots & \frac{\partial T_2}{\partial g_M} \\ . & . & \dots & . \\ \frac{\partial T_M}{\partial g_1} & \frac{\partial T_M}{\partial g_2} & \dots & \frac{\partial T_M}{\partial g_M} \end{bmatrix}_{M\times M} \tag{9}$$

Since temperature calculation at any given time is independent of future heat source values, the upper diagonal terms in Equation 9 become zero. For the linear problem considered here, the application of Duhamel's theorem with constant heat source assumption over each time step, the **X** matrix is simplified as[14]

$$\mathbf{X}=\begin{bmatrix} \nabla\phi_0 & 0 & 0 & 0 & \dots & 0 \\ \nabla\phi_1 & \nabla\phi_0 & 0 & 0 & \dots & 0 \\ \nabla\phi_2 & \nabla\phi_1 & \nabla\phi_0 & 0 & \dots & 0 \\ . & . & . & . & . & . \\ \nabla\phi_{M-1} & \nabla\phi_{M-2} & . & . & \dots & \nabla\phi_0 \end{bmatrix}_{M\times M} \tag{10}$$

where $\nabla\phi_j\equiv\phi_{j+1}-\phi_j$ and ϕ_j is the temperature rise associated with a unit step increase in the internal heat source, i.e., $G(t)=1$ in the heat conduction problem (Equations 1). The temperature rise ϕ_j is calculated by solving these equations with the Crank–Nicolson method.

If the regularization parameter α is known, Equation 2 can be minimized with respect to **g** and the inverse solution for **g** is obtained from Equation 8, since the sensitivity coefficient matrix **X** and $\mathbf{H}_1^T\mathbf{H}_1$ are available from Equations 10 and 4, respectively.

Now the question arises regarding the choice of the optimal value of the regularization parameter α that minimizes the modified sum-of-squares error equation (Equation 2). This matter is discussed in the next section.

Generalized cross-validation approach

In this work, the optimal regularization parameter α is defined as the one that minimizes the sum-of-squares error between

Notation

- **A** Global influence matrix
- **G** True strength of the internal surface heat source vector
- **g** Estimated strength of the internal surface heat source vector
- $\mathbf{H}_1$ First-order regularization matrix
- k Thermal conductivity
- S Sum of square error for first-order regularization procedure
- **T** Estimated temperature vector
- V Generalized cross-validation function
- **X** Sensitivity coefficient matrix
- **Y** Measured temperature vector

Greek symbols

- α Regularization parameter
- δ Dirac delta function
- λ Thermal diffusivity
- σ Standard deviation of measurement temperature
- ϕ Temperature vector for unit-step internal plane heat source
- Ω Sum of square error between the heat source function **G** and **g**

true heat source $G(t)$ and estimated heat source $g(t)$:

$$\Omega(\alpha)=(\mathbf{G}-\mathbf{g})^T(\mathbf{G}-\mathbf{g}) \tag{11}$$

but in a real situation, $\Omega(\alpha)$ cannot be computed because the true internal heat source $G(t)$ is unknown. This is where GCV method enters.

The basic approach in the determination of the optimum value of the regularization parameter α with the GCV method is as follows:

First determine the value of α_{opt} that minimizes the function $V(\alpha)$:[6,8]

$$V(\alpha)=\frac{\frac{1}{M}[\mathbf{Y}-\mathbf{A}(\alpha)\mathbf{Y}]^T[\mathbf{Y}-\mathbf{A}(\alpha)\mathbf{Y}]}{\left[\frac{1}{M}T_r(\mathbf{I}-\mathbf{A}(\alpha))\right]^2} \tag{12}$$

where $T_r(\bullet)$ is the trace of a matrix (i.e., the sum of the diagonals), and the matrix $\mathbf{A}(\alpha)$ is a global influence matrix that will be discussed later.

If α_{opt} determined in this manner is indeed the optimal value of α, it should also be the optimal value of α_{opt} that minimizes Equation 11. Craven and Wahba[6] and Golub[8] have proved that minimizing $V(\alpha)$ is essentially the same as minimizing $\Omega(\alpha)$. The validity of such a result will also be shown by numerical experiments in the Results and Discussion section.

Therefore, the optimum value of the regularization parameter, α_{opt}, is determined from Equation 12 and used in Equation 8 to obtain the inverse solution. The problem now is reduced to that of determining α_{opt} from Equation 12. This is done in the following manner. The first step in the analysis is to develop an explicit expression for the computation of the global influence matrix $\mathbf{A}(\alpha)$ appearing in Equation 12. The matrix $\mathbf{A}(\alpha)$, which relates the measurement data $\mathbf{Y}$ to the estimated temperature $\mathbf{T}$, is defined by

$$\mathbf{T}=\mathbf{A}(\alpha)\mathbf{Y} \tag{13}$$

If we assume $\mathbf{g}_0=\mathbf{T}_0=0$, then Equation 7 reduces to

$$\mathbf{T}=\mathbf{X}\mathbf{g} \tag{14}$$

Introducing Equation 8 into Equation 14, we obtain

$$\mathbf{T}=\mathbf{X}[\mathbf{X}^T\mathbf{X}+\alpha\mathbf{H}_1^T\mathbf{H}_1]^{-1}\mathbf{X}^T\mathbf{Y} \tag{15}$$

A comparison of Equations 13 and 15 reveals that

$$\mathbf{A}(\alpha)=\mathbf{X}[\mathbf{X}^T\mathbf{X}+\alpha\mathbf{H}_1^T\mathbf{H}_1]^{-1}\mathbf{X}^T \tag{16}$$

The value of $\mathbf{A}(\alpha)$ computed from Equation 16 is introduced into Equation 12, and the cubic interpolation is used to minimize $V(\alpha)$ to obtain α_{opt}. In this scheme, $V(\alpha)$ defined by Equation 12 is evaluated for consecutive decreasing (or increasing) values of α until $V(\alpha)$ starts to increase. This value of α, together with its three previous values, are used to determine the four unknown coefficients in the cubic representation of $V(\alpha)$. The resulting functional form of $V(\alpha)$ is then used to compute α_{opt} by setting $dV(\alpha)/d\alpha=0$. The optimal value of α_{opt} established in this manner is used in the least squares method to find the heat source function $g(t)$ that minimize Equation 2.

Results and discussion

To illustrate the application and the usefulness of the GCV method, we consider two specific examples involving the prediction of the timewise variation of the strength of a plane surface heat source, located at the midpoint of a plate, from the knowledge of transient temperature recordings taken at the boundary surface. Initially the plate is at zero temperature, and for time $t>0$, both boundaries are kept insulated. We have chosen a triangular variation over time for the source strength in the first example and a sinusoidal variation in the second example. In both of these examples, the measurement time step is taken as 0.06.

Numerical example 1

Consider a slab of thickness $L=1$. The final time is taken as $t_f=1.8$ and the timewise variation of the strength of the internal plane heat source $G(t)$ located at $x=0.5$ is defined as

$$G(t)=\begin{cases} 0 & 0<t<0.3 \\ t-0.3 & 0.3\le t<0.9 \\ 1.5-t & 0.9\le t\le 1.5 \\ 0 & 1.5<t \end{cases} \tag{17}$$

which represents a triangular variation over time.

In finite differencing with space increment $dx=0.02$, the time increment is chosen as $dt=0.03$ instead of $dt=0.06$ in order to improve the accuracy of computations. In these calculations, all properties are taken as unity. A random noise level of $\omega\sigma$ was added to the simulated exact temperature to generate the measured temperature data, i.e.,

$$Y_{\text{measured}}=Y_{\text{exact}}+\omega\sigma \tag{18}$$

where σ is the standard deviation of measurement errors and is taken as $\sigma=0.001$ and the values of ω are calculated randomly by the IMSL subroutine DRNNOR,[15] which uses normal distribution errors. In the present calculation, the value of ω is chosen over the range $-2.576<\omega<2.576$, which represents the 99% confidence bound for the measurement temperature. The maximum temperature rise in this example is 0.36; therefore $\sigma=0.005$ represents about 1.4% error to the maximum temperature rise.

To show the validity of the GCV method, we use cubic interpolation to determine the optimal value of regularization parameter α_{opt} that minimizes $V(\alpha)$ defined by Equation 12. Similarly, we use cubic interpolation to determine the optimal value of regularization parameter α_{opt} that minimizes $\Omega(\alpha)$ defined by Equation 11. They are in close agreement. To illustrate this matter, in Figure 2 we present plots of $\Omega(\alpha)$ and $V(\alpha)$ *versus* α. This shows that the value of α_{opt} determined from the minimization of $V(\alpha)$ can be used as the α_{opt} needed in the inverse analysis.

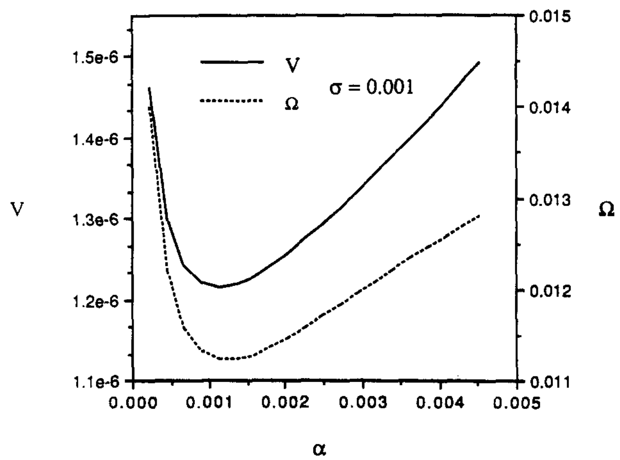

Figure 2 Variation of Ω and V with parameter α for Example 1 for $\sigma=0.001$

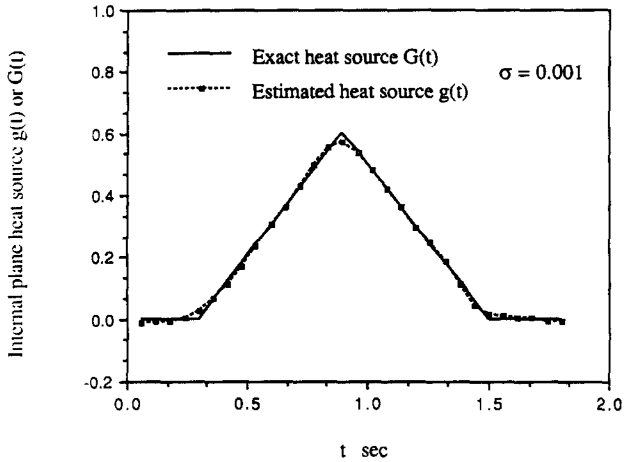

Figure 3 Internal plane heat source for Example 1 for $\sigma=0.001$ ($\alpha_{opt}=1.13\times10^{-3}$)

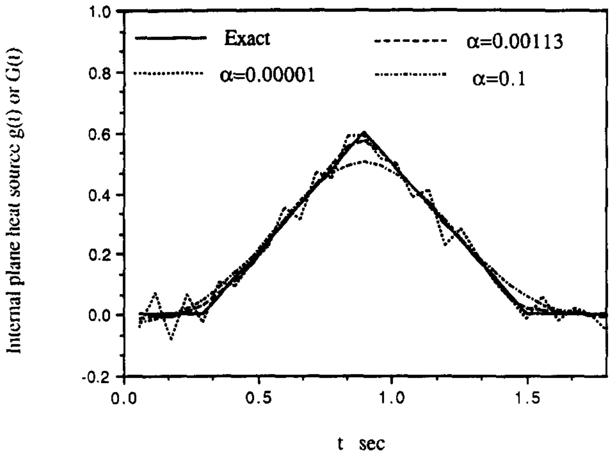

Figure 4 The effectiveness of α to the inverse solution for $\sigma=0.001$

Figure 3 shows a plot of the generation function $g(t)$ determined by the inverse analysis compared with the exact value of $G(t)$ for a standard deviation $\sigma=0.001$. The agreement between the estimated and exact values of the source function is excellent, i.e., the maximum error in the inverse solution including the deterministic and the stochastic errors is under 8%. In these calculations, the optimal value of the regularization parameter α_{opt} determined from the minimization of the function $V(\alpha)$ was $\alpha_{opt}=1.13\times10^{-3}$.

The choice of α is critical to the inverse solution, as shown by Figure 4. In this figure we notice that if α is too small the inverse solution will oscillate (see dotted line) and if α is too large the inverse solution will deviate from exact solution too much (see chain dotted line). Only when $\alpha=\alpha_{opt}$ is the best solution obtained (see dashed line).

To examine the effects of the measurement errors, the experiment was repeated with a larger value of σ, i.e., $\sigma=0.005$. Figure 5 shows that the computed results for $V(\alpha)$ are not exactly the same as for $\Omega(\alpha)$, but they are still in the same range; besides, despite a large increase in the standard deviation, the results are consistent with those given by Trujillo and Busby.[13] The resulting inverse solution with $\alpha_{opt}=8.99\times10^{-3}$ is shown in Figure 6. As expected, increasing the measurement errors decreases the accuracy of the inverse solution.

Numerical example 2

The second example is also for a slab as considered in Example 1, but the timewise variation of the heat source is taken in the form

$$G(t)=\begin{cases}0 & 0<t<0.3\\ \sin\left(\dfrac{[t-0.3]}{0.6}\Pi\right) & 0.3\le t\le 1.5\\ 0 & 1.5<t\end{cases}\tag{19}$$

which represents a sinusoidal variation over time. The space and time increment and properties are the same as those used in Example 1. The maximum temperature rise in this example is 0.38; therefore, $\sigma=0.005$ represents about 1.3% error to the maximum temperature rise.

The resulting $\Omega(\alpha)$ and $V(\alpha)$ for a standard deviation $\sigma=0.001$ are shown in Figure 7, while the inverse solution is shown in Figure 8. The optimal value of regularization parameter α_{opt} was determined as $\alpha_{opt}=2.21\times10^{-4}$. Similar results for $\sigma=0.005$ ($\alpha_{opt}=1.71\times10^{-3}$) are shown in Figures 9 and 10.

The above numerical experiment illustrates that minimizing $V(\alpha)$ is essentially the same as minimizing $\Omega(\alpha)$ for moderate measurement errors. When the measurement errors are large, the optimal values of the regularization parameter α_{opt} for $V(\alpha)$

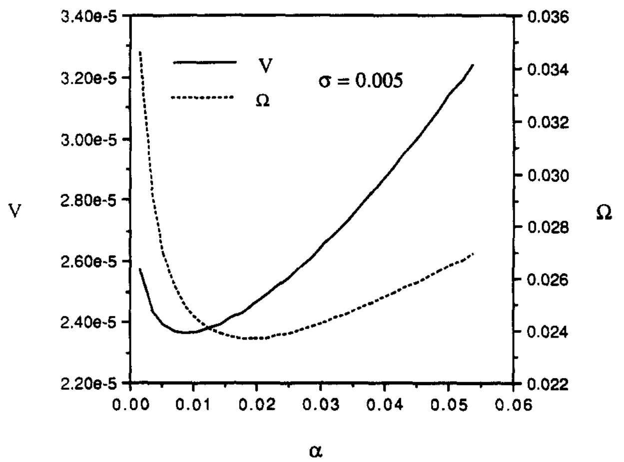

Figure 5 Variance of Ω and V with parameter α for Example 1 for $\sigma=0.005$

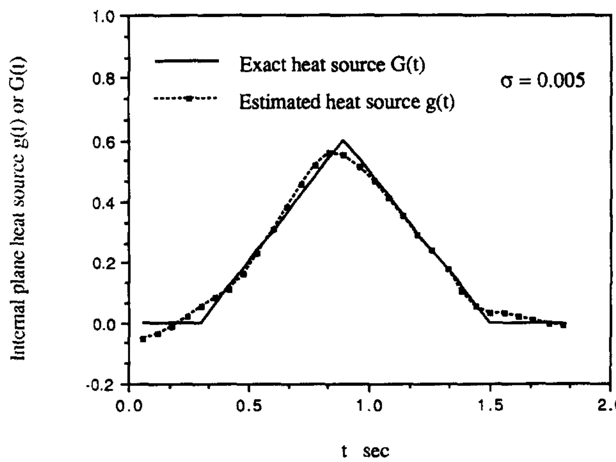

Figure 6 Internal plane heat source for Example 1 for $\sigma=0.005$ ($\alpha_{opt}=8.99\times10^{-3}$)

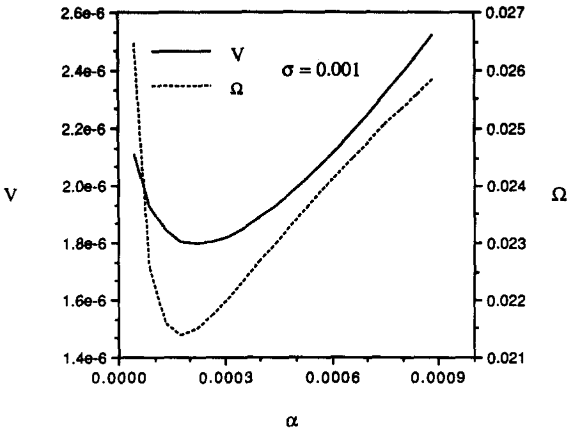

Figure 7 Variation of Ω and *V* with parameter α for Example 2 for $\sigma=0.001$

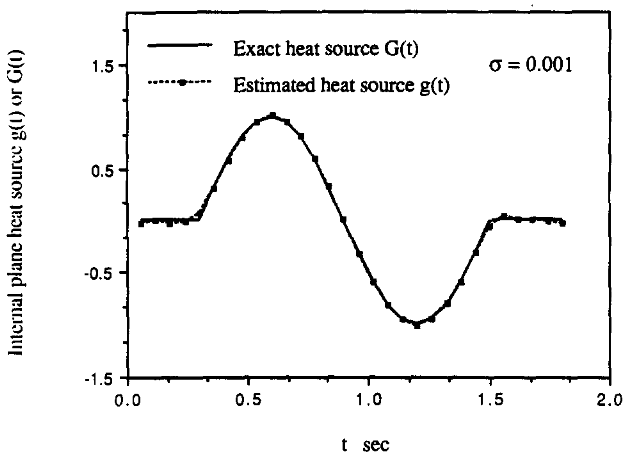

Figure 8 Internal plane heat source for Example 2 for $\sigma=0.001$ ($\alpha_{opt}=2.21\times10^{-4}$)

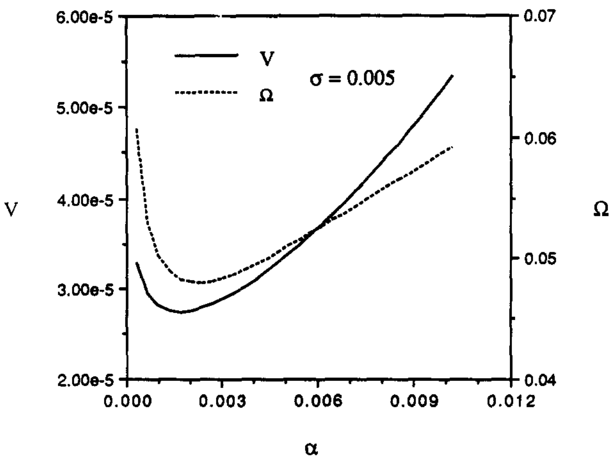

Figure 9 Variation of Ω and *V* with parameter α for Example 2 for $\sigma=0.005$

and $\Omega(\alpha)$ will be deviate, but they are still in the same range and still provide good estimates for the optimal value of the regularization parameter.

When a large number of time steps are required, this algorithm can be arranged as the Sequential Optimal Regularization Method.

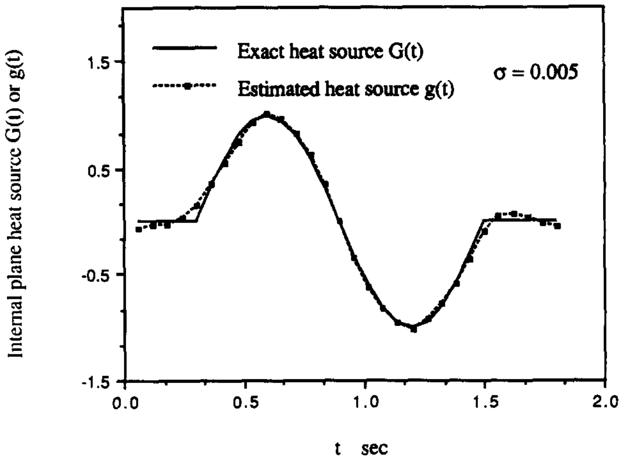

Figure 10 Internal plane heat source for Example 2 for $\sigma=0.005$ ($\alpha_{opt}=1.71\times10^{-3}$)

Conclusions

An efficient inverse method of analysis, utilizing the GCV method to determine the optimal value of regularization parameter α_{opt}, is presented for the estimation of the unknown strength of a plane internal surface heat source $g(t)$ located inside a flat plate.

The advantage of generalized cross-validation (GCV) method lies in the fact that no information other than the measurement data itself is needed. Even with large measurement errors, the method still yields good estimates for the optimal value of the regularization parameter α_{opt}.

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