Combined Function Specification-Regularization Procedure for Solution of Inverse Heat Conduction Problem

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The inverse heat conduction problem involves the calculation of surface heat flux and/or temperature histories from transient, measured temperatures inside solids. This paper proposes and investigates a new combined procedure that is based on two different methods: the sequential function specification method originally proposed by Beck and the regularization method used by Tikhonov and others. The combined method uses the sequential feature of the function specification method and the special function minimized in the regularization method. A test case is investigated of a semi-infinite body exposed to a heat flux that is initially zero, has a step increase, and then drops to zero. A wide range of parameters is investigated. The combined procedure is much more computationally efficient than the usual regularization procedure when all of the flux components are found simultaneously and yet the calculated values found by combined method are little different.

I. Introduction

THE inverse heat conduction problem (IHCP) involves the calculation of surface heat flux and/or temperature histories from transient, measured temperatures inside solids. This inverse problem is a mathematically improperly posed problem because the solution does not depend continuously upon the data.

Various conditions to help stabilize this problem have been reported in the literature:

1) Regularized methods, restricting attention to those solutions satisfying certain prescribed global bounds, have been proposed by Miller,[1] Miller and Viano,[2] and Tikhonov and Arsenin.[3]

2) Reproducing kernel methods have been used recently by Manselli and Miller,[4] Murio,[5,6] and Hills and Mullholland.[7] In these procedures, it is possible to restore certain types of continuous dependence on the data by reconstructing a slightly "filtered" image of the unknown.

3) Beck[8-10] has stabilized the IHCP using several future-time temperatures with a least-squares method to calculate components of the heat flux at a given time. Herein, this method is called the sequential function specification method.

4) By replacing the heat conduction equation with an approximately hyperbolic one, Weber[11] has obtained a well-posed problem for which numerical procedures are already available.

The methods mentioned above, except Refs. 5, 6, and 8-11 are whole domain in the sense that they utilize all of the data to estimate simultaneously the heat flux components. Thus, if the solution is needed over a long period of time, the dimension of the matrices and the number of computations involved increase accordingly.

In contrast, the method proposed by Murio[5,6] leads very naturally to a step-by-step algorithm. After computing the corresponding inverse kernel by solving one small system of equations, the numerial solution is obtained by discrete convolution against the data, with a minimum of computation.

In the sequential methods proposed by Beck[8-10] only a limited number of future time steps are used and only one component of the heat flux vector is found at each step. In these methods, a functional form of the future heat flux is assumed.

In this paper, a new sequential method is introduced by combining the regularization method[1,3] and the function specification method.[8,9] The purpose here is to investigate this method and to compare it with the function specification and regularization methods.

In Sec. II, the problem is presented with the corresponding discrete approximation, together with a detailed description of the new algorithm. Section III shows the results of extensive numerical computations analyzing the solution error as a function of the number of future data temperatures and the regularizing parameter corresponding to exact and noisy data. A comparison with the classical whole domain regularization technique by Tikhonov[3] is also included. Section IV gives a summary and some conclusions.

II. Description of the Problem

A semi-infinite slab is considered to illustrate the method. After obtaining a measured transient temperature history $Y(t)$ at some interior point $x=E$, it is desired to recover the boundary heat flux $q(t)$.

Linear heat conduction with constant thermal properties is considered. Without loss of generality, the problem is normalized by using dimensionless quantities.

The problem in dimensional terms is

$$\frac{\partial T}{\partial t}=\alpha\frac{\partial^2 T}{\partial x^2};\quad 0<x<\infty,\ t>0 \tag{1a}$$

$$T(E,t)=Y(t);\quad t>0 \tag{1b}$$

$$T(x,t)\text{ is bounded as } x\to\infty \tag{1c}$$

$$T(x,0)=T_0;\quad 0<x<\infty \tag{1d}$$

Presented as Paper 84-0491 at the AIAA 22nd Aerospace Sciences Meeting, Reno, NV, Jan. 9-12, 1984; received March 5, 1984; revision received Jan. 3, 1985.

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where t is the time, x the distance measured from the heated surface, α the thermal diffusivity, and T_0 the initial uniform temperature. The objective is to estimate the surface heat flux history $q(t)$, given the interior temperature measurements at $x=E$ and denoted $Y(t)$.

The surface heat flux is related to $T(x,t)$ by

$$q(t) = -k\frac{\partial T}{\partial x}\bigg|_{x=0} \tag{1e}$$

The above problem can be made dimensionless by defining

$$T^+(x^+,t^+) \equiv (T-T_0)/(q_0E/k) \tag{2a}$$

$$Y^+(t^+) = (Y-T_0)/(q_0E/k) \tag{2b}$$

$$x^+ \equiv x/E \tag{2c}$$

$$t^+ \equiv \alpha t/E^2 \tag{2d}$$

$$q^+ \equiv q/q_0 \tag{2e}$$

where q_0 is a nominal value of the surface heat flux. Hence, Eq. (1) can be given as

$$\frac{\partial T^+}{\partial t^+} = \frac{\partial^2 T^+}{\partial (x^+)^2};\quad 0<x^+<\infty,\ t^+>0 \tag{3a}$$

$$T^+(1,t^+) = Y^+(t) \tag{3b}$$

$$T^+(x^+,t^+) \text{ is bounded as } x^+ \to \infty \tag{3c}$$

$$T^+(x^+,0) = 0;\quad 0<x^+<\infty \tag{3d}$$

Also, the surface heat flux equation (1e) can be made dimensionless by

$$q^+(t^+) = -\frac{\partial T^+}{\partial x^+}\bigg|_{x^+=0} \tag{4}$$

For convenience in the remainder of the paper, the dimensionless forms in Eqs. (3) and (4) are used with the + superscripts omitted.

It is well known that Eq. (3) is equivalent to the Volterra integral equation of the first kind,

$$T(1,t) - T_0 = \int_0^t q(s)\frac{\partial \phi(1,t-s)}{\partial t}\mathrm{d}s \tag{5}$$

where $\phi(1,t)$ is the temperature response at $x=1$ for a unit step rise of the surface heat flux at $t=0$.

In a more abstract setting, Eq. (5) can be written as

$$\boldsymbol{T} = \boldsymbol{A}\boldsymbol{q}$$

where $\boldsymbol{T}$ is a vector of values of the elements of Eq. (5), $\boldsymbol{A}$ a square lower triangular matrix, and $\boldsymbol{q}$ a vector of the elements of the heat flux q. Assuming that all the functions involved are L_2 functions on some bounded interval of interest, it is natural also to assume that the unknown function $q(t)$ satisfies an L_2 error bound of the form

$$\|Aq(t) - Y(t)\| \le \epsilon \tag{6a}$$

where the L_2 norms for the continuous and discrete cases are given, respectively, by

$$\|x(t)\| = \left[\int_{t_{\min}}^{t_{\max}} x^2(t)\mathrm{d}t\right]^{1/2} \tag{6b}$$

$$\|x\| = \left[\sum_{n=n_{\min}}^{n=n_{\max}} x_n^2\right]^{1/2} \tag{6c}$$

The discrete case contains a sum of squares.

In order to help stabilize the inverse problem, it is assumed that the unknown function $q(t)$ itself satisfies a known prescribed L_2 bound

$$\|q\| \le E' \tag{7}$$

If $q(t)$ satisfies Eqs. (6) and (7), it also satisfies

$$\|Aq(t) - Y(t)\|^2 + (\epsilon/E')^2\|q(t)\|^2 \le 2\epsilon^2$$

The approximation for the function $q(t)$ is chosen to minimize

$$\|Aq - Y\|^2 + \alpha\|q\|^2,\quad \alpha \equiv (\epsilon/E')^2 \tag{8}$$

where α is called the regularization parameter. This is called a zeroth-order regularization criterion.[14] Another regularization criterion involves first differences of the q elements; in many cases, the results from zeroth- and first-order regularization are similar.[14]

Equation (5) can be approximated at time t_M by

$$T_M = \sum_{n=0}^{M-1} \hat{q}_n \Delta\phi_{M-n} + q_M\Delta\phi_0;\quad q_0 \equiv 0 \tag{9}$$

where

$$T_M = T(M\Delta t) \tag{10a}$$

$$\Delta\phi_i = \phi[(i+1)\Delta t] - \phi(i\Delta t) \tag{10b}$$

$$q_n = q[(n-\tfrac{1}{2})\Delta t] \tag{10c}$$

The caret on q_n denotes a previously estimated value of a heat flux component. The only unknown in Eq. (9) is q_M, which is to be estimated in a sequential manner.

The temperature at times $(M+j)\Delta t$ $(j=0,1,2,\ldots)$ can be given by

$$T_{M+j} = \sum_{n=0}^{M-1} \hat{q}_n\Delta\phi_{M-n+j} + q_M\Delta\phi_j + \ldots + q_{M+j}\Delta\phi_0 \tag{11}$$

The heat flux at time $(M+i-\tfrac{1}{2})\Delta t$ $(i=1,2,\ldots)$ may be expressed as

$$q_{M+i} = A_0 + A_1 i + A_2 i^2 + \ldots + A_\eta i^\eta \tag{12}$$

and the coefficient A_0, which is equal to q_M, is to be found; η is a parameter that can be varied by the analyst. If $\eta=0$, the heat flux is constant, and, if $\eta=1$, there is a linear variation of the surface heat flux.

Assuming that the maximum value of j in Eq. (11) is equal to $r-1$, then it is required, taking into account Eq. (8) in discrete form, that

$$S_r = \sum_{j=0}^{r-1}(T_{M+j} - Y_{M+j})^2 + \alpha\sum_{j=0}^{r-1} q_{M+j}^2 \tag{13}$$

be made a minimum with respect to $A_0, A_1, \ldots, A_\eta$. To obtain a solution, r must be at least as large as $\eta+1$ and, in order to introduce some least-squares smoothing, it is necessary that $r \ge \eta+2$. (Stolz's method[12] is obtained if $\alpha=0$ and $r=1$ or even if $\alpha=0$ and $r=\eta+1$.) Equation (13) uses r future temperatures to obtain the single heat flux component q_M.

Differentiation of Eq. (11) with respect to A_p gives the set of linear equations

$$\sum_{j=0}^{r-1}(T_{M+j} - Y_{M+j})C_{0j} + rA_0 = 0,\quad p=0 \tag{14a}$$

and

$$\sum_{j=0}^{r-1}(T_{M+j}-Y_{M+j})C_{pj}+\alpha\sum_{j=1}^{r-1}j^p q_{M+j}=0, \quad p=1,2,\ldots,\eta \quad (14b)$$

where

$$C_{pj}=\sum_{\ell=0}^{j}\ell^p\Delta\phi_{j-\ell}; \quad p=0,1,2,\ldots,\eta \quad (15)$$

This set of equations is equivalent to

$$\{\beta_{R,0p}+r\}A_0+\left\{\beta_{R,1p}+\alpha\sum_{j=1}^{r-1}j^{p+1}\right\}A_1+\ldots$$

$$+\left\{\beta_{R,\eta p}+\alpha\sum_{j=1}^{r-1}j^{p+\eta}\right\}A_\eta=S_{Rp}, \quad p=0,1,2,\ldots,\eta \quad (16)$$

where,

$$\beta_{R,sp}=\beta_{R,ps}=\sum_{j=0}^{r-1}C_{sj}C_{pj}; \quad \begin{matrix}s=0,1,\ldots,\eta\\ p=0,1,\ldots,\eta\end{matrix} \quad (17)$$

and

$$S_{Rp}=\sum_{j=0}^{r-1}Y_{M+j}C_{pj}-\sum_{n=0}^{M-1}\left(q_n\sum_{j=0}^{r-1}\Delta\phi_{M-n+j}C_{pj}\right); \quad q_0\equiv 0 \quad (18)$$

The method works as follows. After Δt, α, η, and r are chosen ($r\geq\eta+2$), the set of $\eta+1$ equations given by Eq. (16) is solved for A_0. Next the right-hand side of Eq. (16) is updated and solved again. Notice that the inverse matrix is computed only once and its order is given by the value of $\eta+1$. Thus, for $\eta=0$ (piecewise constant solution), there is just one linear equation with one unknown and, if $\eta=1$ (piecewise linear solution), a system of two linear equations with two unknowns is obtained.

III. Numerical Results: Discussion

In order to test the accuracy of the method, approximate reconstruction of a surface heat flux $q(t)$ is investigated for a semi-infinite body exposed to a heat flux of value 1 between $t=0.2$ and 0.6 and of value 0 at other times.

The exact temperature data for this problem are given by

$$T(t)=\phi(1,t-0.2)-\phi(1,t-0.6)$$

where

$$\phi(x,t)=\frac{2}{\pi}\sqrt{t}\exp\left(-\frac{x^2}{4t}\right)-x\,\mathrm{erfc}\left(\frac{x}{2\sqrt{t}}\right), \quad t>0$$

$$=0, \quad t<0$$

When indicated in the paper, the noisy data $Y(t)$ is obtained by adding a random error to T_j, i.e.,

$$Y_j=T_j+\epsilon_j \quad (19)$$

where ϵ_j is a Gaussian random variable of variance σ^2. If σ is equal to zero, there are no random errors. The average perturbation used in this paper is for $\sigma=0.01$ and corresponds to approximately 5% of the maximum true temperature value (about 0.2). In all cases, the time interval of interest is [0,1]. Notice that this interval includes the time periods both before and after heating; it is important to include these periods because the algorithms both anticipate changes in the heat flux and give delayed values.

The top portion of Fig. 1 shows the reconstructed heat flux function obtained with the sequential method and the parameter values $\Delta t=0.05$, $\eta=0$, $r=2$, $\alpha=10^{-4}$, $\sigma=0$ (solid line), and $\sigma=0.01$ (dashed line). The lower portion of Fig. 1

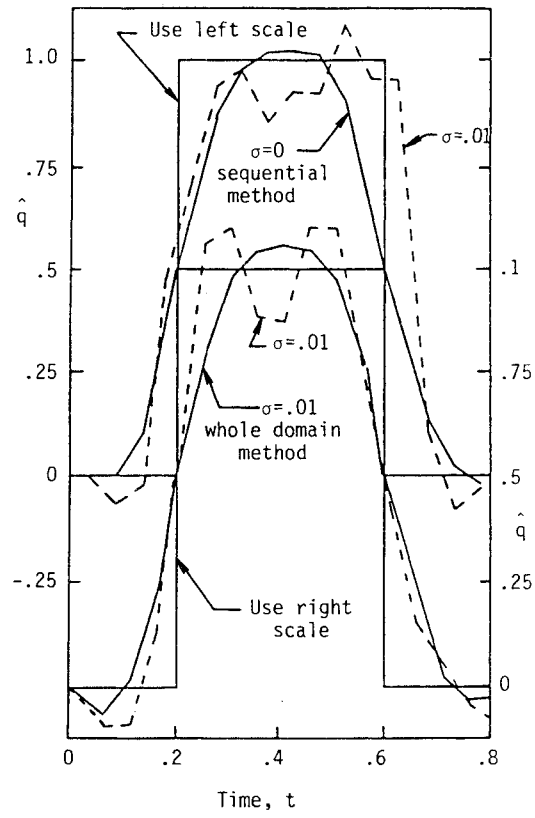

Fig. 1 Reconstructed heat flux function using sequential and whole domain methods with $\Delta t=0.05$, $\eta=0$, $r=2$, and $\alpha=0.0001$.

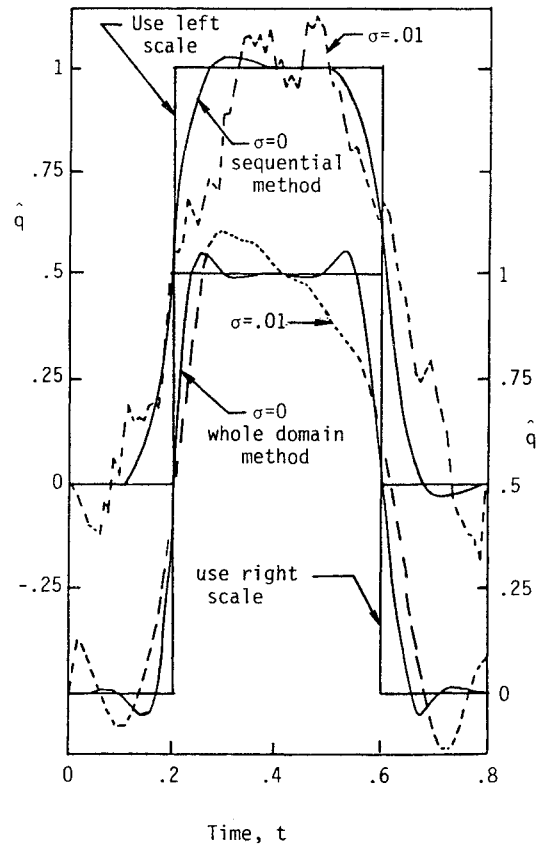

Fig. 2 Reconstructed heat flux function using sequential and whole domain methods with $\Delta t=0.01$, $\eta=1$, $r=13$, and $\alpha=0.0001$.

was obtained using the whole domain regularizer method and the same values for Δt, α, and σ.

Figure 2 corresponds to the same problem with $\Delta t = 0.01$, $\eta = 1$, $r = 13$, $\alpha = 10^{-4}$, $\sigma = 0$, and $\sigma = 0.01$ for the sequential method and the same values of Δt, α, and σ for the whole domain method.

If the discretized computed heat flux component is denoted $\hat{q}_i$ and the true component is q_i, in order to measure the error, the sample root mean square norm is introduced; it is given by

$$\mathbb{S} = \left[\frac{1}{n}\sum_{i=1}^{n}(\hat{q}_i - q_i)^2\right]^{1/2}, \quad n = \frac{1}{\Delta t} \tag{20}$$

The norms of the errors associated with the sequential (s) and whole domain (g) methods in Figs. 1 and 2 are summarized in Table 1. (1s is for the sequential case of Fig. 1 and 1g is for the whole domain case, etc.)

For $\Delta t = 0.05$ (Fig. 1), the sequential method behaves better, but for $\Delta t = 0.01$ (Fig. 2), the whole domain regularization method is clearly superior. However, even in this very difficult case, the sequential method is still very competitive. Furthermore, the savings in computation are enormous and the sequential procedure can be extended to the nonlinear case much more efficiently. The nonlinear case would require a finite difference or element procedure such as described in Ref. 15.

In order to draw conclusions and make further comparisons, it is necessary to estimate the sensitivity of the method to random errors.

If the expected values $[E(\cdot)]$ and variances $[V(\cdot)]$ of the family $\{\epsilon_i\}_{i=1}^{n}$ of random variables associated with the discrete version of Eq. (19) satisfy[13]

$$E(\epsilon_i) = 0, \quad i = 1,2,\ldots,n$$

$$E(\epsilon_i, \epsilon_j) = 0, \quad i \neq j$$

$$V(\epsilon_i) = \sigma^2, \quad i = 1,2,\ldots,n$$

then the theoretical mean squared error of $\hat{q}_i$ is

$$E[(\hat{q}_i - q_i)^2] = E\{[\hat{q}_i|_{\sigma\neq 0} - E(\hat{q}_i|_{\sigma=0})]^2\} + [q_i - E(\hat{q}_i|_{\sigma=0})]^2 = V(\hat{q}_i) + \mathfrak{D}^2 \tag{21}$$

The $\mathfrak{D}^2$ term is the square of deterministic error or bias error and is obtained for zero errors in the data. The deterministic error is due to the algorithms themselves; temporary heat flux assumptions and the regularization term in Eq. (8) contribute to the bias. The value of $\mathbb{S}$ given by Eq. (20) for large n approaches the theoretical value given by Eq. (21).

For the sequential method it can be shown that the estimators $\hat{q}_i$ are linear functions of the measured temperatures and thus one can write[14]

$$\hat{q}_i = \sum_{k=-m_i}^{r-1} D_k Y_{i+k-1} \tag{22}$$

Consequently, it follows that[13,14]

$$V(\hat{q}_i) = \sigma_q^2 = \sum_{k=-m_i}^{r-1} D_k^2 \sigma^2 \tag{23}$$

This statement shows that the variance of the estimated heat flux is proportional to σ^2 and is independent of the error distribution.

A measure of the sensitivity to random measurement errors is given by

$$s_q = \left[\frac{1}{n}\sum_{i=1}^{n}(\hat{q}_i|_{\sigma\neq 0} - \hat{q}_i|_{\sigma=0})^2\right]^{1/2} \tag{24}$$

For large n values, the value of s_q^2 approaches the value $V(\hat{q}_j)$.

The inverse heat conduction algorithms have the effect of reducing the sensitivity to random input errors as measured by Eq. (23) or (24) at the expense of increasing $\mathfrak{D}$, which is a measure of the deviation from the true input heat flux. The best choices of α and r provide an optimal balance between the theoretical values of $V(\hat{q}_j)$ and $\mathfrak{D}^2$. Instead of these theoretical values, the numerically computed values of $\mathbb{S}$ and s_q are given.

A summary of some results for $\Delta t = 0.05$ and $\eta = 0$ is displayed in Fig. 3. The $\mathbb{S}$ values are shown vs the number of future times r. The lowest curve is for $\alpha = 0\text{-}10^{-8}$ and $\sigma = 0$. The $\alpha = 10^{-6}$ result is almost the same. The $\alpha = 10^{-4}$ curve for $\sigma = 0$ starts high and drops to a minimum near $r = 4$. The $\sigma = 0.01$ curve for $\alpha = 10^{-4}$ (dashed line) is almost the same as for $\sigma = 0$. The $\alpha = 0\text{-}10^{-6}$ and $\sigma = 0.01$ curve is also dashed, but starts much higher than the $\sigma = 0$ curve for small r; after $r = 4$, there is little difference. The upper curves of Fig. 3, which are for $\alpha = 1$ and 0.01, are of little interest because the resolution is very poor. For this case of $\Delta t = 0.05$ and $\sigma = 0.01$, the optimal choices (which is at the minimum of $\mathbb{S}$) for r and α are 4 and 10^{-4}, respectively. The conditions for $r = 4$ and $\alpha = 0\text{-}10^{-6}$ will also give near optimal results. Notice that this includes the function specification method or, equivalently, the Beck procedure,[8,10] which has $\alpha = 0$.

As r increases above $r = 4$ in Fig. 3 for $\alpha = 10^{-4}$ and for both $\sigma = 0$ and 0.01, the $\mathbb{S}$ value increases. This is the opposite behavior of s_q/σ for $\Delta t = 0.05$ and $\eta = 0$ shown by the left curve of Fig. 4. In the latter figure, increasing r has the effect of reducing the sensitivity to measurement errors. Figures 3 and 4 illustrate the tradeoff between deviation from the true curve (Fig. 3) and reduction of sensitivity to random errors (Fig. 4).

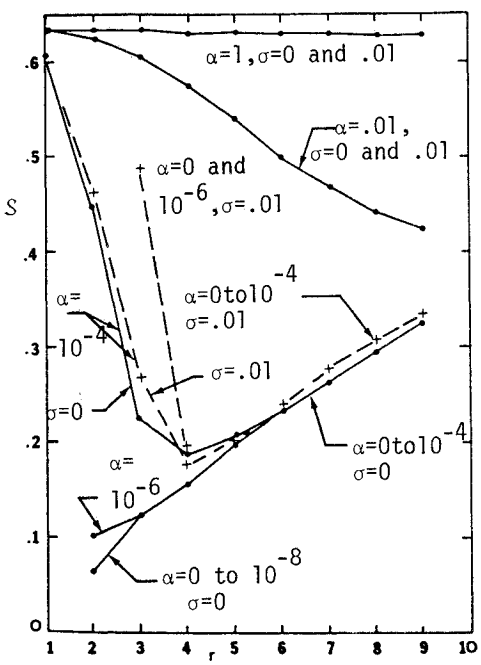

Fig. 3 Estimated total error for $\Delta t = 0.05$ and $\eta = 0$.

Table 1 Root mean square norms of errors

Fig.	$\sigma = 0$	$\sigma = 0.01$
1s	0.1882	0.1761
1g	0.2531	0.2989
2s	0.1789	0.2305
2g	0.1641	0.1827

The same problem of determining the surface heat flux is also investigated for the smaller time step of $\Delta t = 0.01$. Both the constant heat flux assumption ($\eta = 0$) and the linear heat flux assumption ($\eta = 1$) are considered. A plot of S vs r is given in Fig. 5. The lowest curves and the two on the left are for errorless data ($\sigma = 0$). The curves on the upper right are for $\sigma = 0.01$ as well as for $\sigma = 0$. For $\sigma = 0.01$, the optimal choice (defined as minimum S) for $\eta = 0$ is $\alpha = 0\text{-}10^{-4}$ with $r = 15$. Since the $\alpha = 0$ case is the same as for Beck procedure,[8,10] the regularized results are little different. It also happens for $\eta = 1$ and $\sigma = 0.01$ that the minimum S in Fig. 5 is only slightly less (0.235 vs 0.245) than the $\eta = 0$ case. The optimal result for $\eta = 1$ and $\sigma = 0.01$ is obtained for $\alpha = 10^{-4}$ and $r = 13$. Hence, for $\eta = 1$ (linear q approximation), the regularized result is better than for $\alpha = 0$ (Beck procedure).

The sensitivity to errors for the $\Delta t = 0.01$ case can be investigated by using Fig. 4. Notice that the $\Delta t = 0.01$ case is about two orders of magnitude more sensitive than for $\Delta t = 0.05$. Also, the $\eta = 1$ case for $\Delta t = 0.01$ is generally much more sensitive to random errors than $\eta = 0$. For larger r (about 14), the results for various α tend to collapse for both $\eta = 0$ and 1. In such cases, there is little improvement over the $\alpha = 0$ (i.e., Beck[8,10]) procedure. Notice also that in Fig. 5 whenever the $\eta = 1$ results are better than the $\eta = 0$ results in terms of the minimum bias S, in Fig. 4 the opposite is true in terms of sensitivity to errors.

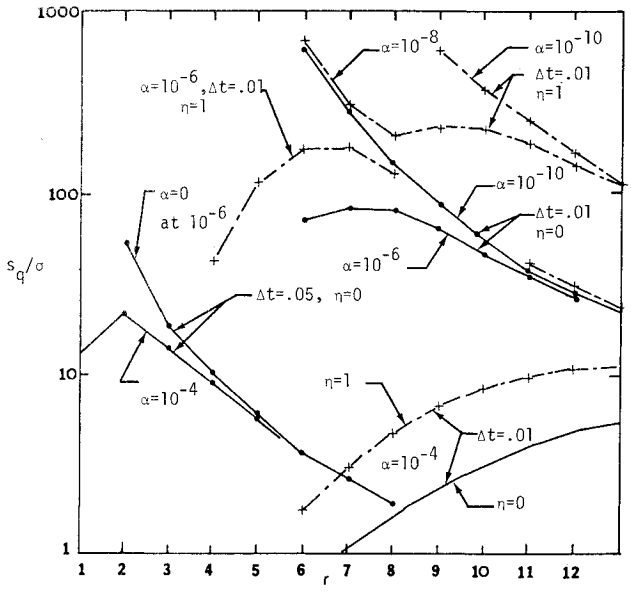

Fig. 4 Normalized estimated standard deviation of errors in q.

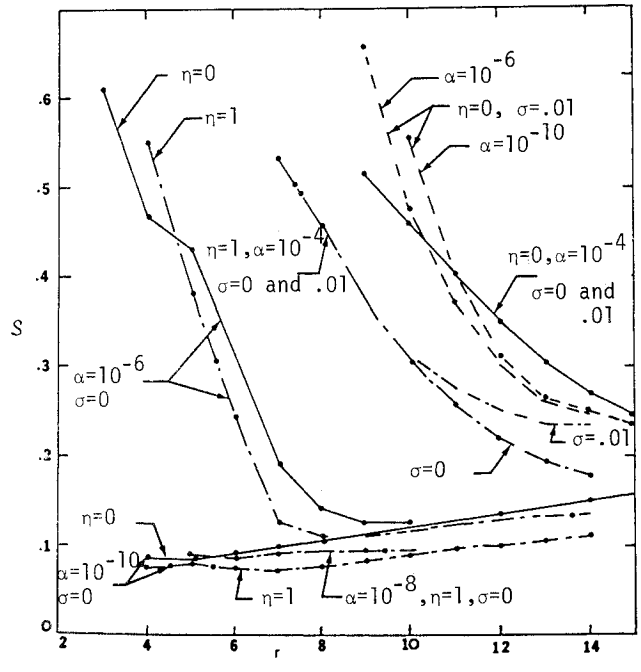

Fig. 5 Estimated total error for $\Delta t = 0.01$ for $\eta = 0$ and 1.

IV. Summary and Conclusions

A combined sequential function specification and classical whole-domain regularization technique is derived and investigated. The method is sequential and thus is much more computationally efficient than the whole-domain regularization method.

A test case is investigated of a semi-infinite body subjected to a heat flux that is zero for all times except for a finite time interval when it is a constant. Such a curve has the difficult characteristics of an abrupt rise and an equally abrupt drop. A number of parameters are varied, including time step size, number of future time steps, type of heat flux approximation, and regularization parameter.

The combined sequential method is compared with the classical whole-domain regularization method. In some cases the combined method is better and in others the whole-domain regularization is better; but even so, the combined method results are very competitive. This is important because the combined procedure is much more computationally efficient.

For a dimensionless time step of 0.05, a constant heat flux assumption ($\eta = 0$), and random errors corresponding to $\sigma = 0.01$, the combined method is slightly better than the sequential function specification method. The same is true for the case of the small dimensionless time step of 0.01. In the case of both the combined and sequential function specification methods, reduction of the time step from 0.05 to 0.01 increased the optimal number of future time steps from about 4 to 14.

The case of a linear approximation of the surface heat flux is compared with that of a constant heat flux. The former is considerably more sensitive to measurement errors, but is better in some cases than the latter.

A general conclusion is that the sequential function specification method can be improved upon by various methods. In most cases, the improvements are relatively modest. Consequently, the sequential function specification with a constant heat flux approximation remains a viable procedure.

An important result of this paper is the methodology for comparison of methods. See Ref. 14 for more discussion of this point.

Acknowledgment

The work of the first author was supported in part by the National Science Foundation under Grant MEA81-21499.

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