International Journal of Thermophysics, Vol. 21, No. 2, 2000

An Inverse Analysis to Estimate Relaxation Parameters and Thermal Diffusivity with a Universal Heat Conduction Equation[1]

D. W. Tang[2] and N. Araki[2, 3]

This paper presents an inverse analysis for simultaneous estimation of relaxation parameters and thermal diffusivity with a universal heat conduction model by using temperature responses measured at the surface of a finite medium subjected to pulse heat fluxes. In the direct analysis, the temperature responses in a finite medium subjected to a pulse heat flux are derived by solving the universal heat conduction equation. The inverse analysis is performed by a nonlinear least-squares method for determining the two relaxation parameters and thermal diffusivity. Here, the nonlinear system of algebraic equations resulting from the sensitivity matrix is solved by the Levenberg–Marquardt iterative algorithm. The inverse analysis is utilized to estimate the relaxation parameters and the thermal diffusivity from the simulated experimental non-Fourier temperature response obtained by direct calculation.

KEY WORDS: inverse analysis; Levenberg–Marquardt algorithm; pulse heating; relaxation parameters; thermal diffusivity; universal heat conduction model.

1. INTRODUCTION

Temperature responses under ultra-high-speed heating or at ultra-low temperature exhibit behavior not predicted by thermal diffusion theory. Models have been developed to describe these experiments [1–3]. To extend these

---

[1] Paper presented at the Fifth Asian Thermophysical Properties Conference, August 30–September 2, 1998, Seoul, Korea.

[2] Department of Mechanical Engineering, Faculty of Engineering, Shizuoka University, Hamamatsu 432-8561, Japan.

[3] To whom correspondence should be addressed.

0195-928X/00/0300-0553$18.00/0

models from the macro- to the microscales, Tzou [4] introduced phase lags to the Fourier law and developed a dual-phase-lag model:

$$\mathbf{q}(\mathbf{r}, t) + \tau_q \frac{\partial \mathbf{q}}{\partial t} = -\lambda \left[\nabla T(\mathbf{r}, t) + \tau_T \frac{\partial}{\partial t}(\nabla T) \right] \tag{1}$$

where τ_q and τ_T are the phase lags (the relaxation times) of the heat flux and temperature gradient, respectively; thus provides a macroscopic description of the microscopic effects. Applying some ideas of the Jeffreys model for shear waves in liquids to the description of heat flux propagation in solids, Joseph and Preziosi [2] developed the same form of heat flux equation as Eq. (1), but with some parameters from the theory of liquids. They described the microstructural effects by a relaxation function (heat-flux kernel), and separated it into fast and slow modes which correspond to two relaxation times. Equation (1) and the conservation equation without a heat source lead to a description of transient heat conduction with the following generalized equation:

$$\frac{1}{a}\frac{\partial T}{\partial t} + \frac{\tau_q}{a}\frac{\partial^2 T}{\partial t^2} = \nabla^2 T + \tau_T \frac{\partial}{\partial t}(\nabla^2 T) \tag{2}$$

Comparing Eq. (2) with microscopic models shows that, if the two relaxation times are formulated properly in terms of microscopic quantities for different materials, this macroscopic model gives exactly the same heat conduction equation as the microscopic models. The comparisons can also provide a microscopical physical understanding of the two new introduced relaxation parameters. For dielectric crystals, τ_q is the relaxation time for the momentum-nonconserving processes and τ_T is of the same order as the relaxation time for the normal processes conserving momentum in the phonon system. For metals, τ_q represents the relaxation behavior of electron thermal-wave conduction, while τ_T represents the effect of phonon–electron interaction. The Fourier thermal diffusion law and the Cattaneo–Vernotte thermal wave law are two special cases of this generalized model for $\tau_T = \tau_q = 0$ and $\tau_T = 0$, respectively [1]. This model can provide microscopic descriptions for almost all heat conduction behaviors by giving appropriate relaxation parameters and thermophysical properties. Conversely, these parameters can be determined by fitting the solution of this generalized equation to the measured temperatures.

The generalized model is used to treat the heat conduction problem in a finite medium exposed to a pulse heat flux with a Gaussian temporal profile, corresponding to an actual short heat pulse. The analytical solution of the generalized heat conduction equation is derived by the Green's function method and a finite integral transform technique [5, 6].

In this work, by using this temperature solution, we perform the inverse analysis by a nonlinear least-squares method for determining the two relaxation parameters and thermal diffusivity from a given temperature response. The nonlinear system of algebraic equations resulting from the sensitivity matrix is solved by the Levenberg–Marquardt iterative algorithm. The inverse analysis is utilized to estimate the relaxation parameters and the thermal diffusivity from the simulated experimental non-Fourier temperature response obtained by direct calculation.

2. DIRECT PROBLEM

In the direct problem, the temperature field in a finite rigid slab of thickness L with an initial temperature distribution $T(x,0)=T_0$ (x is the direction along the thickness), constant thermal properties, and insulated boundaries is determined. From $t=t_0$, the front surface ($x=0$) of this slab is heated uniformly by a pulse heat flux with a Gaussian temporal profile as follows:

$$I(t)=\frac{I_0}{\sqrt{\pi t_p}}\exp\left[-\left(\frac{t}{t_p}\right)^2\right] \tag{3}$$

where t_p is the characteristic time and I_0 is the total energy per unit cross section of the heat flux. According to refs. 5 and 7, the conduction heat transfer in the slab can be modeled as a one-dimensional problem with an energy source $Q(x, t)$ near the surface,

$$Q(x,t)=\frac{I_0}{t_p\delta\sqrt{\pi}}\exp\left(-\frac{x}{\delta}-\left(\frac{t}{t_p}\right)^2\right) \tag{4}$$

where δ is the absorptive depth of heating energy. Then the equation of conservation of energy is given by

$$Q(x,t)-\frac{\partial q}{\partial x}=c_p\rho\frac{\partial T}{\partial t} \tag{5}$$

Combining Eq. (5) with Eq. (1) in one-dimensional form leads to the following governing equation for the problem:

$$\frac{1}{a}\frac{\partial T}{\partial t}+\frac{\tau_q}{a}\frac{\partial^2 T}{\partial t^2}$$
$$=\frac{\partial^2 T}{\partial x^2}+\tau_T\frac{\partial}{\partial t}\left(\frac{\partial^2 T}{\partial x^2}\right)+\frac{1}{\lambda}\left[Q(x,t)+\tau_q\frac{\partial Q}{\partial t}\right] \qquad (0\leqslant x\leqslant L,\ t>t_0) \tag{6}$$

For the considered situation, the boundary and initial conditions are taken as

$$\partial t(x, t)/\partial x|_{x=0} = \partial T(x, t)/\partial x|_{x=L} = 0 \tag{7}$$

$$\partial T(x, t)/\partial x|_{t=t_0} = 0, \qquad T(x, t)|_{t=t_0} = T_0 \tag{8}$$

By using the Green's function method, the temperature distribution is obtained as [5]

$$V(x, t) = R(1 - e^{-L/\delta}) \int_{t_0}^{t} (1 - e^{-(t-\tilde{t})/\tau_q}) \left(1 - \frac{2\tau_q \tilde{t}}{t_p^2}\right) e^{-(\tilde{t}/t_p)^2} \, d\tilde{t}$$

$$+ \begin{cases} 4R \sum_{k=1}^{N} \dfrac{1-(-1)^k e^{-L/\delta}}{\chi\sqrt{\beta}} \cos(\lambda_k x) \displaystyle\int_{t_0}^{t} e^{-[1+\lambda_k^2 a\tau_T](t-\tilde{t})/2\tau_q} \\ \quad \times \sin\left[\dfrac{\sqrt{\beta}\,(t-\tilde{t})}{2\tau_q}\right]\left(1 - \dfrac{2\tau_q \tilde{t}}{t_p^2}\right) e^{-(\tilde{t}/t_p)^2} \, d\tilde{t}, \qquad \beta > 0 \\ 4R \sum_{k=N}^{\infty} \dfrac{1-(-1)^k e^{-L/\delta}}{\chi\sqrt{-\beta}} \cos(\lambda_k x) \displaystyle\int_{t_0}^{t} e^{-[1+\lambda_k^2 a\tau_T](t-\tilde{t})/2\tau_q} \\ \quad \times \sinh\left[\dfrac{\sqrt{-\beta}\,(t-\tilde{t})}{2\tau_q}\right]\left(1 - \dfrac{2\tau_q \tilde{t}}{t_p^2}\right) e^{-(\tilde{t}/t_p)^2} \, d\tilde{t}, \qquad \beta < 0 \end{cases}$$

where

$$\lambda_k = k\pi/L \tag{10a}$$

$$\chi = 1 + (\lambda_k \delta)^2 \tag{10b}$$

$$\beta = 4\lambda_k^2 a\tau_q - [1 + \lambda_k^2 a\tau_T]^2 \tag{10c}$$

and N is the point at which β changes from positive to negative with increase in the value of k.

3. INVERSE PROBLEM

The inverse problem is concerned with the simultaneous estimation of relaxation parameters and thermal diffusivity from the measured temperature response at the surface of the specimen exposed to a heat flux with a temporal profile defined by Eq. (3). The experimental conditions are described as those in the direct problem and assumed to be known exactly, while the measured temperature data may contain random errors.

In the inverse analysis, the parameters to be estimated are the relaxation parameters τ_q and τ_T and thermal diffusivity a. The problem is to compute the estimates of these parameters which will minimize the least-squares norm of experimental temperature values and the expected values from Eq. (9). If the vectors of experimental and expected values of the temperature responses are $\mathbf{V}_\mathrm{E}$ and $\mathbf{V}$, respectively, the least-squares norm can be written in matrix form as [8]

$$S(\beta) = [\mathbf{V}_\mathrm{E} - \mathbf{V}(\beta)]^T [\mathbf{V}_\mathrm{E} - \mathbf{V}(\beta)] = \mathbf{F}^T\mathbf{F} \tag{11}$$

where

$$[\mathbf{V}_\mathrm{E} - \mathbf{V}(\beta)]^T = [V_E(t_1) - V(t_1;\beta),\dots, V_E(t_m) - V(t_m;\beta)] \tag{12}$$

$$\beta^T = [\tau_q, \tau_T, a] = [z_1, z_2, z_3] \tag{13}$$

$V_E(t_i)$ are the measured temperatures at time t_i, and m is the total number of measurements. The estimated temperatures $V(t_i;\beta)$ at time t_i and at the measurement locations are obtained from the solution (9) by using the estimation for the unknown vector β. The following condition should be satisfied in order to minimize the least-squares norm:

$$\nabla_\beta S(\beta) = 2[-\nabla_\beta \mathbf{V}^T(\beta)][\mathbf{V}_\mathrm{E} - \mathbf{V}(\beta)] = 0 \tag{14}$$

Here, the sensitivity matrix is

$$\Im(\beta) = [\nabla_\beta \mathbf{V}^T(\beta)]^T = \begin{bmatrix} \Im_{1\tau_q} & \Im_{1\tau_T} & \Im_{1a} \\ \Im_{2\tau_q} & \Im_{2\tau_T} & \Im_{2a} \\ \vdots & \vdots & \vdots \\ \Im_{m\tau_q} & \Im_{m\tau_T} & \Im_{ma} \end{bmatrix} \tag{15}$$

where the sensitivity coefficients are given by

$$\Im_{i\tau_q} = \frac{\partial V(t_i;\tau_q,\tau_T,a)}{\partial \tau_q} \tag{16a}$$

$$\Im_{i\tau_T} = \frac{\partial V(t_i;\tau_q,\tau_T,a)}{\partial \tau_T} \tag{16b}$$

$$\Im_{ia} = \frac{\partial V(t_i;\tau_q,\tau_T,a)}{\partial a} \tag{16c}$$

where $i = 1, 2,\dots, m$. To solve the nonlinear system of algebraic equations (14), the Levenberg–Marquardt iterative algorithm [9] is used, which combines the steepest descent and Newton methods. This algorithm is based upon expanding $\mathbf{V}(\beta)$ in a Taylor series to the first-order terms and adding the Levenberg–Marquardt parameter μ. We obtain the following formula to compute the search direction for the parameters β:

$$\beta^{n+1} = \beta^n - (\mathfrak{J}^T\mathfrak{J} + \mu^n \mathbf{I})^{-1}\, \mathfrak{J}^T \mathbf{F} \tag{17}$$

where $\mathfrak{J}$ is the Jacobian matrix with elements defined as

$$\mathfrak{J}_{ij} = \partial V(t_i, \beta)/\partial z_j, \qquad i = 1, 2, \ldots, m, \quad \text{and} \quad j = 1, 2, 3 \tag{18}$$

$\mathbf{I}$ is the identity matrix, and the superscript n is the iteration index. The solution of the inverse problem starts with a suitable guess β^0, and the iterations are continued until

$$|z_j^{n+1} - z_j^n| < \varepsilon, \qquad j = 1, 2, 3 \tag{19}$$

where ε is a small, positive number.

4. STATISTICAL ANALYSIS

Assuming that the temperature measurement errors are additive, independent in a normal distribution, and have zero means with constant standard deviations σ, the standard deviations of the estimated values are obtained by using the statistical analysis in Ref. 8:

$$\sigma_{\tau_q} = \sigma \sqrt{\frac{A_{22}A_{33} - A_{23}^2}{A}} \tag{20a}$$

$$\sigma_{\tau_T} = \sigma \sqrt{\frac{A_{11}A_{33} - A_{13}^2}{A}} \tag{20b}$$

$$\sigma_a = \sigma \sqrt{\frac{A_{11}A_{22} - A_{12}^2}{A}} \tag{20c}$$

where

$$A = A_{11}A_{22}A_{33} + 2A_{12}A_{13}A_{23} - (A_{11}A_{23}^2 + A_{22}A_{13}^2 + A_{33}A_{12}^2) \tag{21}$$

$$A_{11} = \sum_{i=1}^{m} \mathfrak{J}_{i\tau_q}^2, \qquad A_{22} = \sum_{i=1}^{m} \mathfrak{J}_{i\tau_T}^2, \qquad A_{33} = \sum_{i=1}^{m} \mathfrak{J}_{ia}^2 \tag{22a}$$

$$A_{12} = \sum_{i=1}^{m} \mathfrak{J}_{i\tau_q}\mathfrak{J}_{i\tau_T}, \qquad A_{13} = \sum_{i=1}^{m} \mathfrak{J}_{i\tau_q}\mathfrak{J}_{ia}, \qquad A_{23} = \sum_{i=1}^{m} \mathfrak{J}_{i\tau_T}\mathfrak{J}_{ia} \tag{22b}$$

The 99% confidence intervals for the estimated parameters are given in Ref. 8:

$$\text{Probability}[(z_i - 2.576\sigma_{z_i}) < z_{i,\,\text{exact}} < (z_i + 2.576\sigma_{z_i})] \approx 99\%, \qquad i = 1, 2, 3 \tag{23}$$

5. AN ESTIMATION EXAMPLE

By using the above method, the relaxation parameters and thermal diffusivity can be estimated simultaneously from the values of measured temperature responses under conditions described in the direct problem. In the estimation program, the function is calculated using Eq. (9), the Jacobians are calculated using the formula obtained from the derivatives of Eq. (9) with respect to the parameters, and the nonlinear equations (14) are solved using the subroutine DBCLSJ of IMSL [10].

As an example, a simulated experimental temperature response $V_{\text{experiment}}$ at the front surface ($x = 0$) of a film with a thickness of $L = 8.0 \times 10^{-2}\ \mu\text{m}$ heated by a short pulse of duration $t_p = 2.0$ ps is generated by adding an error term $\omega\sigma$ to the exact temperature V_{exact} computed with Eq. (9),

$$V_{\text{experiment}} = V_{\text{exact}} + \omega\sigma \tag{24}$$

where ω lies in the range $-2.576 \leqslant \omega \leqslant 2.576$ if a 99% confidence interval is assumed for the measured data, which can be randomly generated by using the IMSL subroutine DRNNOR [10]. In this example, the exact temperature response is calculated under the condition

$$\delta = 2.0 \times 10^{-3}\ \mu\text{m}, \qquad t_0 = -8.0\ \text{ps}, \qquad R = 1.0$$

The relaxation times and thermal diffusivity are

$$\tau_q = 10\ \text{ps}, \qquad \tau_T = 0\ \text{ps}, \qquad a = 4.0 \times 10^{-5}\ \text{m}^2 \cdot \text{s}^{-1}$$

and the number of temperature data is $m = 200$. The temperature response and the corresponding sensitivity coefficients are shown in Fig. 1. It is desired that the sensitivity coefficients have large and linearly independent values for obtaining reliable estimations. As seen in this figure, the sensitivity coefficients should satisfy this demand. The initial guesses for the values of relaxation parameters and thermal diffusivity are

$$\tau_q^{(0)} = 20\ \text{ps}, \qquad \tau_T^{(0)} = 1.0\ \text{ps}, \qquad a^{(0)} = 1.0 \times 10^{-4}\ \text{m}^2 \cdot \text{s}^{-1}$$

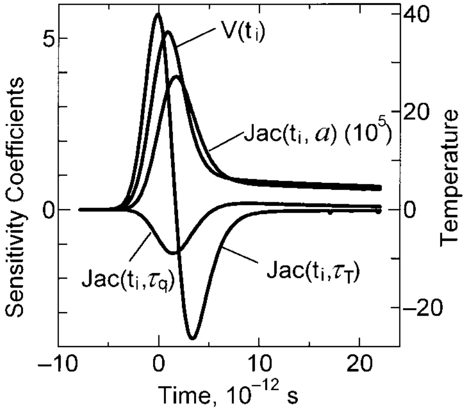

Fig. 1. Dimensionless temperature response and corresponding sensitivity coefficients. Here Jac(t_i, τ_q) $= \Im_{i\tau_q}$, Jac(t_i, τ_T) $= \Im_{i\tau_T}$, Jac(t_i, a) $= \Im_{ia}$.

For the case of $\sigma = 0$, the iteration history for these estimated parameters in the calculation is shown in Fig. 2. As seen in the figure, after more than 200 iterations, the calculated parameters converge to their estimated values and the calculation is finished. The estimated results for various measurement standard errors are listed in Table I. Comparisons with the exact values show that at the lower measurement error of temperature response, reliable estimates can be provided by this method.

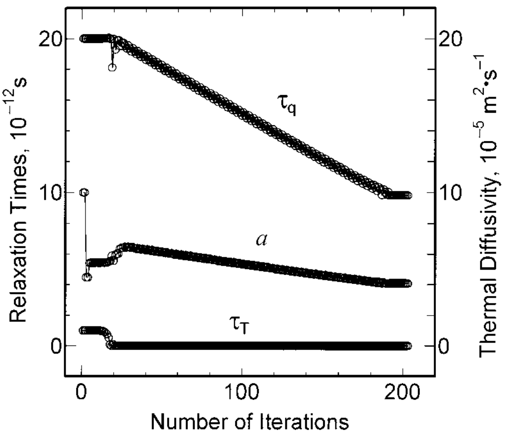

Fig. 2. Iteration process to estimate the parameters from initial guesses ($\sigma = 0$).

Table I. Estimated Results for Various Standard Errors

σ/V_{max}	τ_q (ps)	τ_T (ps)	a ($m^2 \cdot s^{-1}$)
0.0	9,909	0.000	4.096×10^{-5}
0.01	9.822	0.000	4.071×10^{-5}
0.05	8.327	0.000	4.700×10^{-5}
0.1	8.012	0.000	5.113×10^{-5}

REFERENCES

1. M. N. Özisik and D. Y. Tzou, *J. Heat Tansfer* **116**:526 (1994).
2. D. D. Joseph and L. Preziosi, *Rev. Mod. Phys.* **61**:41 (1989).
3. D. Y. Tzou, *Macro- to Micro-scale Heat Transfer: The Lagging Behavior* (Taylor & Francis, Bristol, 1997).
4. D. Y. Tzou, *J. Heat Transfer* **117**:8 (1995).
5. D. W. Tang and N. Araki, in *Proc. 34th Natl. Heat Transfer Symp. Jpn.* (Sendai, 1997), p. 165.
6. D. W. Tang and N. Araki, in *Proc. 35th Natl. Heat Transfer Symp. Jpn.* (Nagoya, 1998), p. 259.
7. D. W. Tang and N. Araki, *J. Phys. D: Appl. Phys.* **29**:2527 (1996).
8. J. V. Beck and K. J. Arnold, *Parameter Estimation in Engineering and Science* (Wiley, New York, 1977).
9. D. W. Marquardt, *SIAM J. Appl. Math.* **11**:431 (1963).
10. IMSL, *User's Manual IMSL MATH/LIBRARY* (Library, Houston, 1987).