PARAMETER ESTIMATION METHOD FOR FLASH THERMAL DIFFUSIVITY WITH TWO DIFFERENT HEAT TRANSFER COEFFICIENTS

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ABSTRACT

Determining thermal diffusivity using flash diffusivity tests at high temperatures is investigated using parameter estimation. One aspect is the development of a method for determining two different heat transfer coefficients, one at the heated face and one at the opposite face. Both simulated exact and experimental data are used to illustrate the procedure. Although the heat transfer coefficients are different, assuming the heat transfer coefficients in the estimation process are the same does not significantly affect the estimates of the thermal diffusivity.

Insight into the estimation of thermal diffusivity and other parameters is obtained from a study of the sensitivity coefficients. Although the thermal diffusivity is the primary parameter of interest, a measured signal proportional to the temperature rise also depends on the heat transfer coefficients and energy input, which are called nuisance parameters (if they are not of interest). As the temperatures increase above 1500°C, the heat losses become very large and greatly influence the temperature response. By using insights from the study of the sensitivity coefficients for each of these parameters, the thermal diffusivity can be estimated despite the large heat losses.

INTRODUCTION

Flash diffusivity methods have been used to determine the thermal diffusivity of solids from low to elevated temperatures [1-6]. However, as the temperature increases, the heat losses from the specimen surfaces rapidly increase, resulting in more difficult analysis of the data. The heat loss from the specimen can be caused by free convection and radiation. If the specimen is in a vacuum, only radiation losses are possible. In both cases, the heat losses can be described by heat transfer coefficients.

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For tests at elevated temperatures (greater than 1500°C), the heat losses can be large and the surface temperatures on either face are quite different. The heat transfer coefficients can also be different in magnitude. However, the heat transfer coefficients on both faces of the specimen are commonly assumed to have the same value[1-6].

This paper investigates the simultaneous estimation of the thermal diffusivity, two heat transfer coefficients (one at $x = 0$ and the other at $x = L$, see Fig. 1) and the input power. The analysis is intended for elevated temperatures and the associated large heat losses. The main parameter of interest is the thermal diffusivity but sometimes the three other parameters must be simultaneously estimated; they are termed nuisance parameters. Parameter estimation techniques are used to estimate these parameters and are described for this problem. Estimating all these parameters simultaneously is deceptively difficult. The correlation between parameters can be very high, which means that simultaneous determination of such parameters can be both difficult and inaccurate. Fortunately, it also means that the number of parameters can be reduced.

An outline of the remainder of the paper is now given. First a mathematical model for this problem is given and followed by the analytical solution. Next the parameter estimation concepts are given and a case with exact data is investigated. The method is then applied to analyze a set of experimental data. The paper ends with conclusions.

MATHEMATICAL MODEL AND SOLUTION

The specimen is modeled as a flat plate of thickness L. A signal proportional to the temperature rise at $x = L$ is measured using noncontact, averaging radiation sensors. In the experimental data used herein, the specimen is about 1 mm in thickness and about 25 mm in diameter. For these conditions, the one-dimensional plate model as shown in Figure 1 is appropriate. The surface at $x = 0$ is assumed to be heated with an instantaneous heat flash at time $t = 0$. (The analysis can be readily modified to treat a finite duration of the pulse.) Heat transfer coefficients of h_1 and h_2 are at the faces at $x = 0$ and L, respectively. The ambient temperature is assumed to be the constant value of T_∞. These heat transfer coefficients can be used to describe the heat loss for both free convection and radiation.

The mathematical model and boundary conditions are

$$\alpha\frac{\partial^2 T}{\partial x^2} = \frac{\partial T}{\partial t} \tag{1}$$

$$-\lambda\frac{\partial T}{\partial x}\Big|_{x=0} = q_0\delta(t) - h_1[T(0,t) - T_\infty] \tag{2}$$

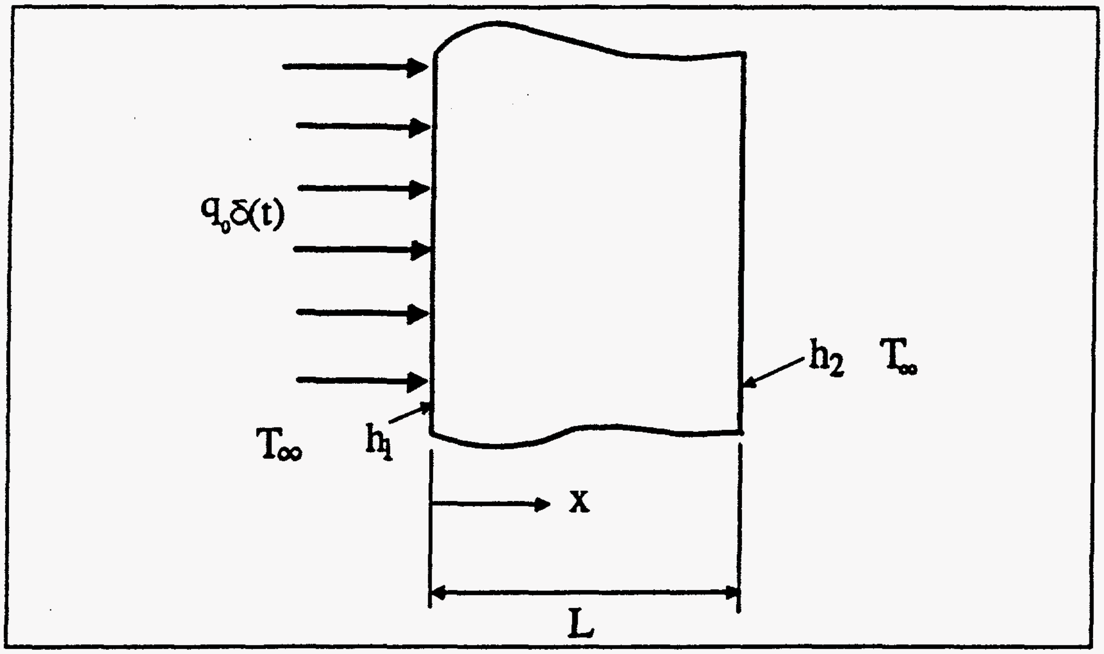

Figure 1. Diagram of a specimen heated by a flash at $x = 0$ and with heat transfer coefficient h_1 at $x = 0$ and heat transfer coefficient h_2 at $x = L$.

$$-\lambda \frac{\partial T}{\partial x}\bigg|_{x=L} = + h_2[T(L,t) - T_\infty] \tag{3}$$

The initial temperature is T_∞. The symbol $\delta(t)$ is the Dirac delta function that is zero everywhere except t near zero and its integral over t is equal to one. The units of the energy input, q_0, are J/m^2. Implicit in eq. (1) is the assumption that the thermal conductivity, λ, does not vary significantly over the temperature range of a particular flash experiment, although it can vary greatly one experiment to another.

An analytical solution of the above problem is a Green's function [7],

$$T(L,t) = T_\infty + \frac{2q_0}{\rho c L}\sum_{m=1}^{\infty} e^{-\eta_m^2 \alpha t/L^2}\frac{C_m}{N_m} \tag{4}$$

$$C_m = \eta_m(\eta_m \cos\eta_m + B_1 \sin\eta_m) \tag{5}$$

$$N_m = (\eta_m^2 + B_1^2)\left[1 + \frac{B_2}{\eta_m^2 + B_2^2}\right] + B_1 \tag{6}$$

The η_m's are eigenvalues found from $\tan\eta_m = \eta_m(B_1 + B_2)/(\eta_m^2 - B_1 B_2)$ where $B_1 = h_1 L/\lambda$ is the Biot number at $x = 0$ and $B_2 = h_2 L/\lambda$ is the Biot number at $x = L$; λ is the thermal conductivity. The thermal diffusivity, the parameter of interest, is denoted α.

One important decision is determining which parameters or groups can be estimated from transient signals at the $x = L$ face. The above solution shows that the temperature rise at L can be expressed as a function of four parameters denoted β_1, β_2, β_3, and β_4 where

$$\beta_1 = \alpha, \quad \beta_2 = \frac{q_0}{\rho c L}, \quad \beta_3 = B_1 = \frac{h_1 L}{\lambda}, \quad \beta_4 = B_2 = \frac{h_2 L}{\lambda} \tag{7}$$

For β_2, three unknowns are included: energy input q_0, density ρ and specific heat c; however, only the parameter β_2 (= $q_0 / \rho c L$) is needed. Since the T rise is proportional to β_2, only a signal proportional to the temperature rise must be measured. The last two parameters, β_3 and β_4, also involve the ratio of unknown quantities, such as h_1 over λ. Although only the thermal diffusivity, α, is often the single desired parameter, the other three groups (or parameters) must also be simultaneously estimated.

PARAMETER ESTIMATION

In these experiments, the measurement errors in the temperature rise (or a signal proportional to it) can be considered additive and unbiased and to have a constant variance. A cost function for these assumptions is the sum of squares. Since the sensitivity coefficients for β_3 and β_4 are correlated, Tikhonov regularization [8] is used, resulting in the sum of squares function for j =1, 2, . ., J measurements,

$$S = \sum_{j=1}^{J} (Y_j - T_j)^2 + \alpha_{Tik}(\beta_3^2 + \beta_4^2) \tag{8}$$

where Y_j and T_j are the measured and calculated temperatures at time t_j and $x = L$; T_j is calculated using the model given by eq. (4). The second term in this equation is called a zeroth order Tikhonov regularization term. The Tikhonov regularization parameter, α_{Tik}, is made sufficiently small that the estimates of the diffusivity are little affected but α_{Tik} is made big enough to allow convergence. Some examples of selecting α_{Tik} is given later.

Estimates of the four parameters are obtained by minimizing eq. (8) by taking the first derivative of S with respect to the parameters β_i (I = 1, 2, 3, 4) and setting each equation equal to zero (see chap. 7, [9] for a complete discussion),

$$\frac{\partial S}{\partial \beta_i} = 2\sum_{j=1}^{J} (Y_j - T_j)(-\frac{\partial T_j}{\partial \beta_i}) + 2\alpha_{Tik}\beta_i\Delta = 0 \tag{9}$$

where $\Delta = 0$ for i =1 and 2 and $\Delta = 1$ for i = 3 and 4. Four simultaneous nonlinear algebraic equations are obtained from eq. (9). The partial derivatives, $\partial T/\partial \beta_i$, in eqs. (9) are called sensitivity coefficients; see [10] for explicit expressions.

Determination of the confidence intervals for the thermal diffusivity is found using the classical statistical procedure with some assumptions regarding the measurement errors. The covariance matrix of the estimates of the parameters is calculated using eq. (7.7.1) of ref. 9. The diagonal term associated with the thermal diffusivity is the variance of the estimated value. Its square root is the estimated standard deviation of the estimated thermal diffusivity. The estimated confidence region is calculated as shown in Sect. 7.7 of ref. 9.

The values of the covariance matrix depend upon the assumptions that are valid for the measurement errors. These assumptions used herein are that the errors are additive, have zero mean (that is, are unbiased), have a constant variance and are first order autoregressive. A method of treating the first order autoregressive errors is given in Sect. 6.9 of ref. 9. These assumptions should be checked by examining the residuals which are simultaneously obtained with the parameter estimates.

Another basic assumption is that the model is correct. If it is not, then a systematic variation (a characteristic bias or "signature") will occur in the residuals that is repeated from test to test. One such imperfection in the model might be the lack of treatment of thermal penetration of the laser flash, causing the initial temperature distribution to be nonuniform.

Ideally uncorrelated measurements errors would be obtained and revealed by the residuals; unfortunately measurement errors are frequently either correlated or biased. Nevertheless it can be stated that the confidence intervals of the thermal diffusivity are certain values, provided the assumptions are valid.

EXACT DATA EXAMPLES

An example with simulated temperatures (correct to six significant figures) is first given. The thickness is 1.0 and the initial temperature is 0.0. The true values of the parameters are α (=β_1) equals 1; $q_0/\rho cL$ (=β_2) equals 1, B_1 (=β_3) equals 0.5 and B_2 (=β_4) equals 0.1. The temperature curve is shown as the upper one in Figure 2. Forty data points are used with dimensionless time steps of $\alpha \Delta t/L^2 = 0.05$. Two sets of initial "guesses" are used. For the first three rows of Table I, all the starting parameter values are correct except the second one which is 0.7 while the true value is 1.0. The last three rows of Table I use the initial "guesses" of 1, 0.7, 0.5 and 0.5. Estimated parameters are denoted b_i and results are shown in Table I for values of the Tikhonov regularization parameter α_{Tik} from 10^{-16} to 10^{-8}. In each convergent case the estimated

TABLE I. RESULTS OF ESTIMATING PARAMETERS USING EXACT DATA

Initial Values of Parameters	α_{Tik}	Estimated b_1	b_2	Parameters b_3	b_4	Std. Dev. s	Thermal Diffusivity Confidence Interval
1, 0.7, 0.5, 0.1	10^{-8}	1.0035	0.9893	0.2810	0.2810	0.167E-4	1.0027 to 1.0042
1, 0.7, 0.5, 0.1	10^{-12}	1.0002	0.9994	0.4932	0.1046	0.257E-6	0.99982 to 1.00056
1, 0.7, 0.5, 0.1	10^{-16}	1.0000	1.0000	0.5000	0.1000	0.268E-8	0.99996 to 1.00004
1, 0.7, 0.5, 0.5	10^{-8}	1.0035	0.9893	0.2810	0.2810	0.166E-4	1.00270 to 1.0042
1, 0.7, 0.5, 0.5	10^{-12}	1.0034	0.9994	0.2859	0.2761	0.109E-5	1.0032 to 1.0036
1, 0.7, 0.5, 0.5	10^{-16}	NONCONVERGENT					
Exact Parameter Values:		1	1	0.5	0.1		

α (that is, b_1) is very near the true value of 1.0. The confidence regions for this parameter are also given by the last pair of numbers. The quantity denoted s is the estimated standard deviation of the measurements, which is an estimate of the standard deviation of the simulated measurements (about 10^{-6}).

For the first row of Table I ($\alpha_{Tik} = 10^{-8}$), the estimated values of the Biot numbers (b_3 and b_4) are both about 0.28, which is near the average of the true values of 0.1 and 0.5. For even smaller values of α_{Tik} shown in the second and third rows of Table I, estimates b_3 and b_4 are quite accurate, indicating that the computational procedure is correct with extremely accurate data and quite different values of β_3 and β_4. The last three rows of Table I show that the estimation process is much more difficult if the initial guesses for β_3 and β_4 are the same value. However, for the cases that do converge (rows 4 and 5) the parameter of interest, the thermal diffusivity, is negligibly affected by the estimates of the last two parameters. Consequently in many cases, it is satisfactory to estimate the thermal diffusivity with the assumption that the two heat transfer coefficients are equal. A reason why there is a tendency for b_3 and b_4 to approach the same value is because the sensitivity coefficients for β_3 and β_4 tend to be correlated. See the below discussion of Figures 2 and 3.

The choice of the Tikhonov parameter may require some experimentation. One concept is to make it as small as possible and yet obtain convergence. Another concept is to choose α_{Tik} so that the estimated standard deviation of the temperatures, s, is about the expected value, which is about 10^{-6}. Reference to Table I shows that $\alpha_{Tik} = 10^{-12}$ satisfies this condition.

The dimensionless temperature rise, Fourier number, and dimensionless modified (by multiplying by β_i) sensitivity coefficients $Z(i)$, i = 1,2,3, 4 are defined by

$$T^+ = \frac{T-T_\infty}{\beta_2}, \quad t^+ = \frac{\alpha t}{L^2}, \quad Z(i) = \frac{\beta_i}{\beta_2}\frac{\partial T}{\partial \beta_i}, \quad i=1,..,4 \tag{10}$$

Dividing Z(i) by β_2 eliminates the dependence of Z(i) upon β_2. Multiplication of $Z(i)$ by β_i gives the modified sensitivities and permits comparison with the temperature rise. Notice that T^+ is equal to $Z(2)$.

Figure 2 displays results for β_3 =0.5 and β_4 = 0.1; $Z(2)$ reaches a maximum value about 0.7 and then starts to decrease with dimensionless time, t^+. The dimensionless sensitivity for the thermal diffusivity, $Z(1)$, is relatively large at early times, reaching a maximum about 0.53 and then decreases to negative values. The Biot number sensitivity coefficients (β_3 and β_4) are smaller in magnitude and correlated (i.e., have the same shape). Since β_3 and β_4 are nuisance parameters, these conditions of small sensitivies and correlation need not significantly affect the estimation of β_1 $(=\alpha)$. It suggests setting β_3 equal to β_4 (and estimating only β_3) will not significantly affect the estimation of β_1. This can be seen by examining the results of Table I.

Since it may not be necessary to estimate independently two Biot numbers, in the next case the Biot numbers are assumed to be equal. Figure 3 shows results for β_3 = β_4 = 10. The magnitude of the β_1 sensitivity coefficient tends to be larger than that of the temperature rise and the β_2 sensitivity coefficient. That is advantageous for estimating β_1. The correlation between *Z(2)* and *Z(3)* (that is, *Z(2)/Z(3)* is nearly a constant) indicates that the simultaneous estimation of β_1, β_2 and β_3 may be difficult. However, regularization may be used to improve the convergence for β_1.

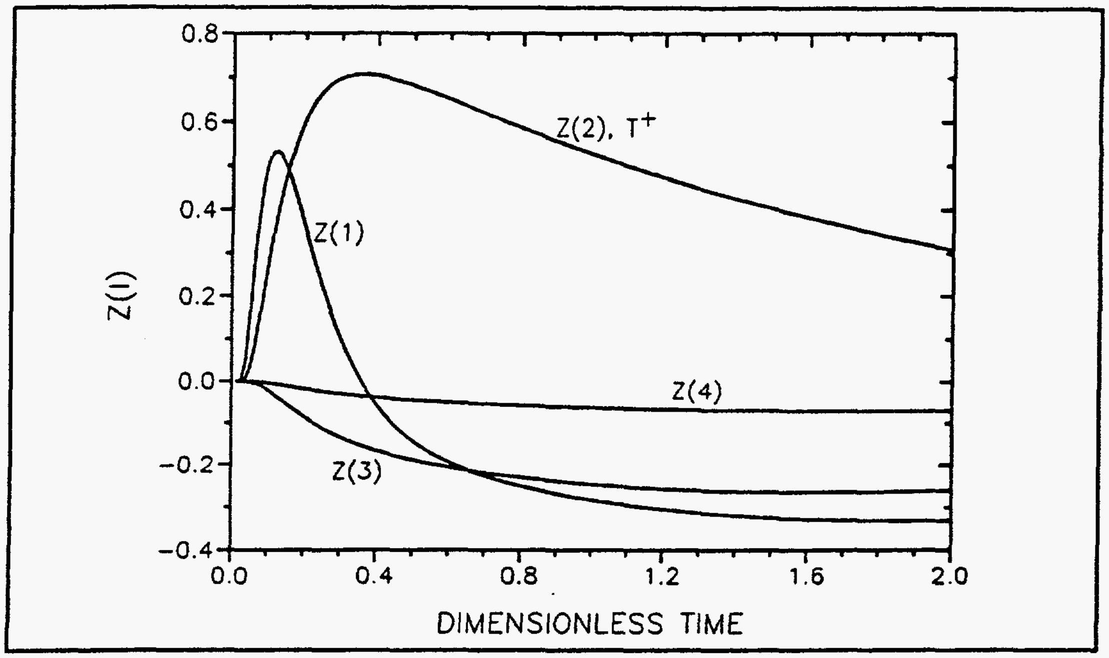

Figure 2. Exact temperature rise and modified sensitivity coefficients for $\alpha = 1$, $\beta_2 = 2q_0/\rho cL = 1$, $\beta_3 = B_1 = 0.5$ and $\beta_4 = B_2 = 0.1$. Values plotted versus dimensionless time, $\alpha t/L^2$.

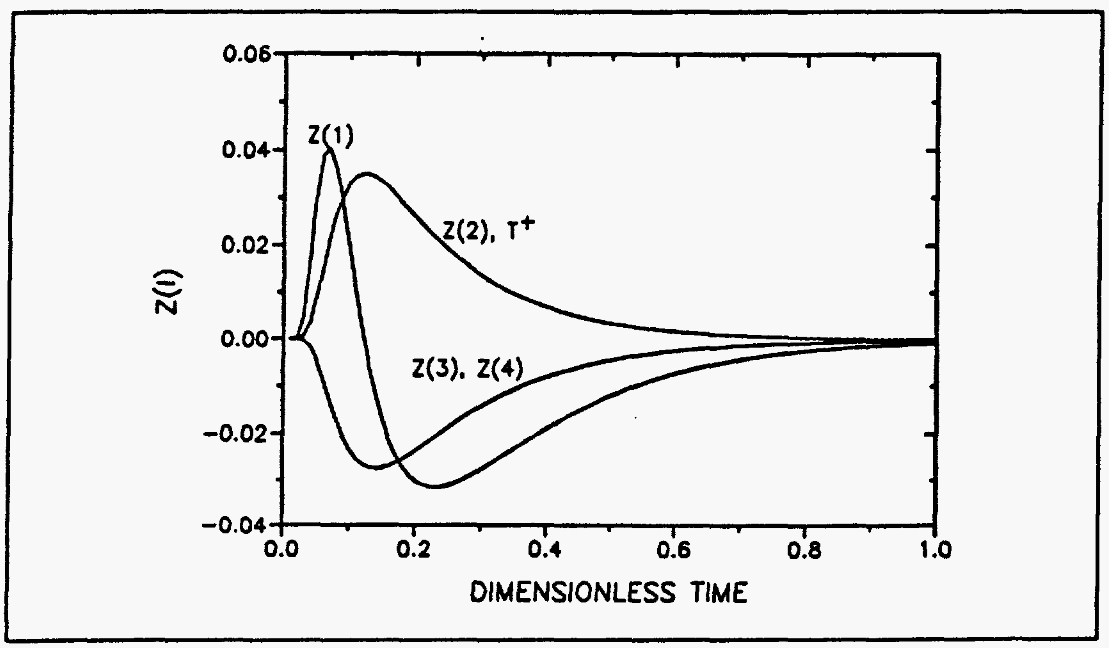

Figure 3. Exact temperature rise and modified sensitivity coefficients for $\alpha = 1$, $\beta_2 = 2q_0/\rho cL = 1$, $\beta_3 = B_1 = 10$ and $\beta_4 = B_2 = 10$. Values plotted versus dimensionless time, $\alpha t/L^2$.

EXPERIMENTAL DATA EXAMPLE

Transient temperatures for carbon bonded carbon fiber insulation (CBCF) at 2000 °C are shown in Figure 4. The temperature response is given in "volts" units. An analysis was performed for estimating the four parameters, (diffusivity, energy input, and the two Biot numbers). Because of the high correlation between the two Biot numbers, Tikhonov regularization using eq. (8) was needed. Using all 472 data points, a range of α_{Tik} values was chosen for the initial estimates of the Biot numbers of $\beta_3 = 12$ and $\beta_4 = 8$. For each α_{Tik} value shown in Table II, the converged values of the two Biot numbers are equal, though different as α_{Tik} is varied. The minimum regularization for α_{Tik} is about 10^9 which is a large numerical value because the magnitude of the "volts" in Figure 4 is large. For smaller α_{Tik} values and the same initial estimates of parameters, the procedure has difficulty converging. The important point is that the α estimates, denoted b_1, are relatively insensitive to changes in the Tikhonov parameter; for example, increasing α_{Tik} by a factor of 1000 increases b_1 by only 15%.

The reason that the two Biot numbers converge to the same values in Table II for a specified α_{Tik} value is the very high correlation in the sensitivity coefficients. Since the two Biot numbers coalesce to the same values, it is reasonable to estimate only three parameters, (α, energy input, and the same Biot number for both surfaces). The estimated parameters are 0.006524 cm²/s, 579,900 and 10.645 for α, energy input and Biot number, respectively. The parameter estimates can be plotted sequentially with time. The sequential values are those that would be obtained if the number of measurements that are used increased one by one until all the data is used. In well-designed experiments and when an appropriate number of parameters are estimated, the sequential estimates should be nearly constant for at least the last half of the experiment duration. For this case, very large variations with time of the sequential parameters is found. The sequential values change so greatly because the energy input and Biot number (β_2 and β_3) sensitivity coefficients are correlated, as indicated by Figure 3. (Figure 3 is for the four parameters but for the case of identical Biot values at $x = 0$ and L, the sensitivity coefficient for the same Biot number on both surfaces is just a factor of two larger than that shown for β_3.) Correlation between two sensitivity coefficients can be determined by dividing one by the other and plotting the result as a function of time. If the ratio is nearly constant, then high correlation exists and fewer parameters should be estimated. The ratio of the second and third sensitivity coefficients is almost a constant in this case. This suggests estimating only two parameters with the Biot number given a few values.

TABLE II. RESULTS OF ESTIMATING PARAMETERS USING EXPERIMENTAL DATA FOR INITIAL VALUES OF $\beta_3 = 12$ AND $\beta_4 = 8$. DATA NOT FILTERED.

		Estimated	Parameters			Std. Dev.
α_{Tik}	b_1	b_2	b_3	b_4	S_{min}	s
10^{12}	0.00738	267600	6.363	6.363	0.217E+9	680.9
10^{10}	0.00676	450700	9.058	9.058	0.120E+9	506.4
10^{9}	0.00662	519500	9.928	9.928	0.1079E+9	480.2
10^{8}	NONCONVERGENT					

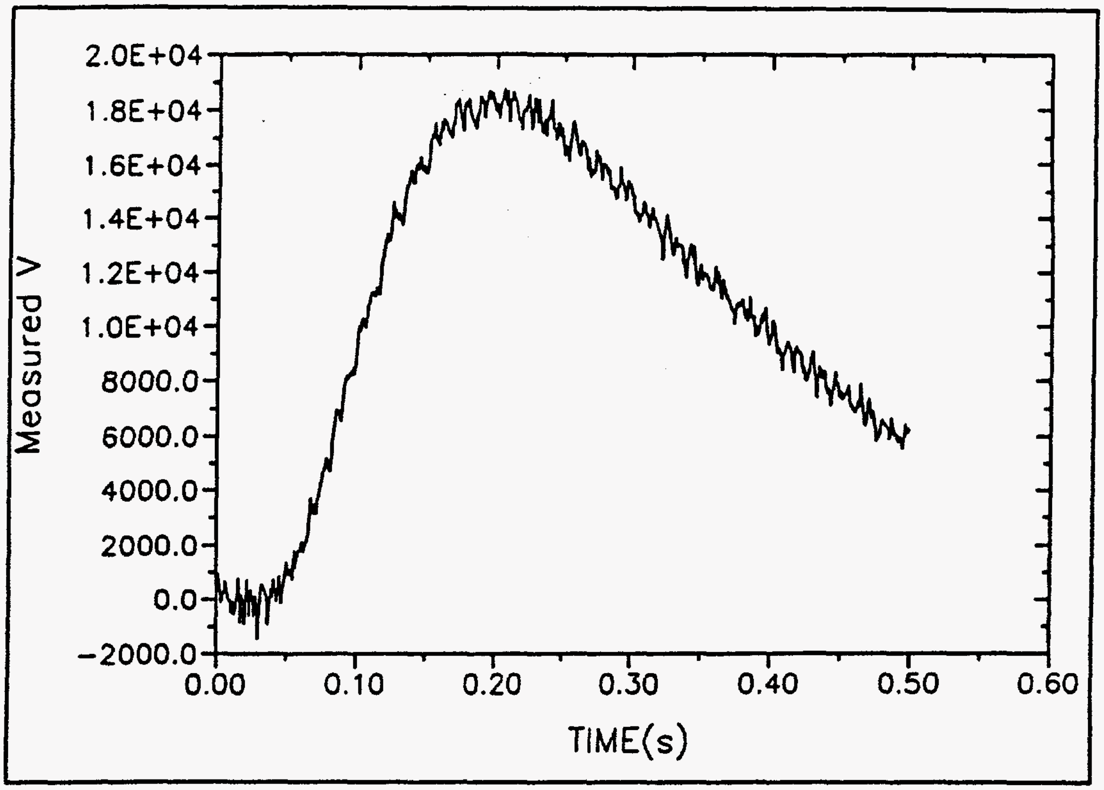

Figure 4. Measured temperature rise (in arbitrary volt units) versus time for CBCF at 2000°C.

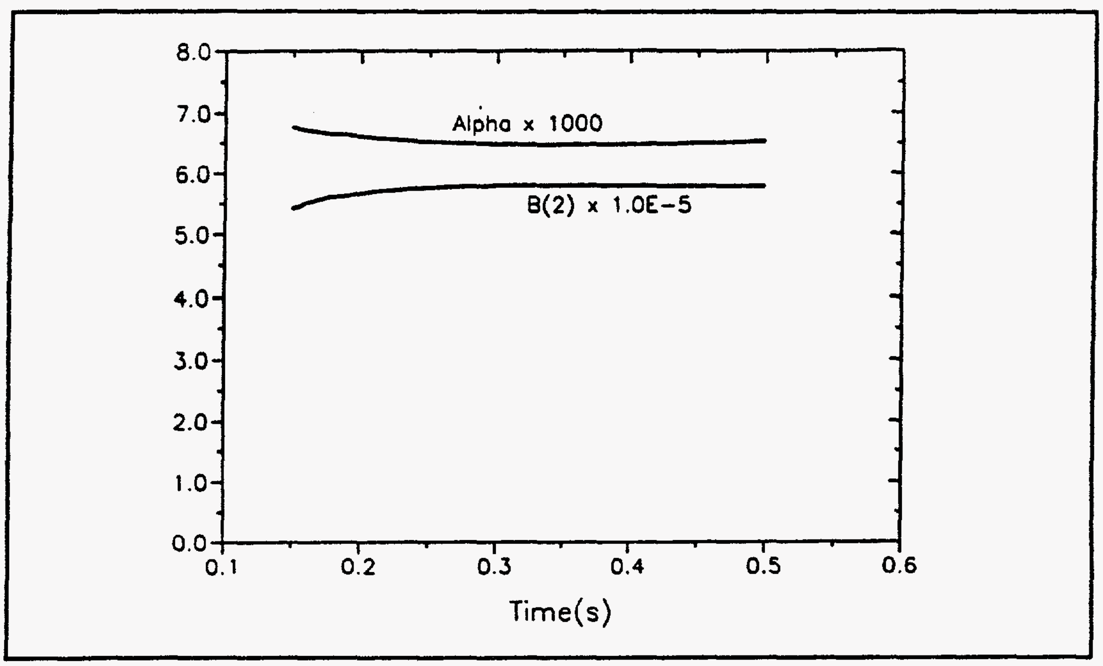

Figure 5. Sequential parameter estimates for CBCF at 2000°C for two parameters: thermal diffusivity and input energy; Biot number = 10.65.

TABLE III. RESULTS OF ESTIMATING β_1 and β_2 FOR SPECIFIED VALUES OF β_3. DATA FILTERED, FIRST TWO MEASUREMENTS DROPPED AND INITIAL TEMPERATURE CORRECTION.

β_3	b_1, cm^2/s	b_2	S_{min}	s	Thermal Diffusivity Confidence Interval
7	0.00720	305700	0.607E+8	359	0.00648 to 0.00791
9	0.00677	444800	0.413E+8	296	0.00636 to 0.00717
10.65	0.00652	578500	0.379E+8	284	0.00618 to 0.00687
12	0.00637	700600	0.386E+8	285	0.00602 to 0.00671
15	0.00611	1013000	0.439E+8	304	0.00572 to 0.00649

Figure 5 shows sequential results for estimating only two parameters, thermal diffusivity and energy input. These results are for the Biot number, β_3, equal to the converged value for three parameters which is 10.65. Before discussing this plot, several points are made. First, the data was filtered at each time by simply using the average of five previous, the measured value at that time and five subsequent measured temperatures. Also the first two measurements were omitted since they seemed to be high and a small correction for a non-zero initial temperature was added. The net effect of the filtering, etc. was negligible upon the parameter estimates shown by Figure 5. Second, filtering is very reasonable to reduce the effects of the periodic noise. The period of this noise is about eleven data points, hence the choice of the filtering region. Third, the estimated values shown in Figure 5 are not greatly affected by the value of the fixed value of β_3. The fourth and final point is that the estimated value of the thermal diffusivity in Figure 5, 0.00652 cm^2/s, is more properly given with a confidence region. Using standard statistical methods and assuming that the measurement errors are first order autoregressive[9] yields the confidence region of 0.00618 to 0.00687 cm^2/s. If the same procedure were used for β_3 equal to 7 to 14, the associated confidence intervals include the above value of 0.00652, shown in Table III.

Returning now to a discussion of Figure 5, the most obvious and satisfactory feature is that the thermal diffusivity and the energy input are nearly constant over a very large time range. This is in contrast to the case of estimating three parameters. The three parameters have large sequential variations because the second and third parameters are highly correlated. See Figure 3 which is for about the same Biot number. Figure 3 also shows that the first two parameters are quite uncorrelated, which is one reason that the sequential values in Figure 4 are nearly constant. One of the difficulties of this analysis for two parameters is that an estimate of β_3 is needed. However, a 114% increase in β_3 from 7 to 15 causes only a 15% drop in the estimated thermal diffusivity. If the β_2 and β_3 parameters were perfectly correlated then changes in β_3 would not affect the thermal diffusivity (β_1). As it is, there is a slight change in the thermal diffusivity. The confidence region of 0.00618 to 0.00687 cm^2/s (or ±5%) is reasonable for measurements at 2000°C if the main source of errors is in the random temperature measurement. For lower temperatures, the Biot numbers are smaller and the correlation between the power and Biot number is decreased. This makes estimation of the three parameters (β_1, β_2 and β_3) easier.

Another important aspect is the examination of the residuals which are the differences between the measured and calculated temperatures. Because of space limitations, they cannot be shown. However, it is sufficient to describe them as increasing from zero at t = 0 to 550 at 0.08s, decreasing to -500 at 0.15s increasing to 550 at 0.3s and finally going down to -600. There is a little fluctuation in the residuals and the data was filtered before analysis . Two observations are made. The residuals are relatively small, with the maximum magnitude about 3% of the maximum temperature rise. This indicates that the model is good. The second observation is that the residuals tend to be correlated and the residuals just less than 0.1s are more significant because the temperatures at those times are small.

CONCLUSIONS

Methods to estimate the thermal diffusivity using data from flash diffusivity tests at elevated temperatures are discussed and illustrated using simulated and experimental data. At elevated temperatures the heat losses from the specimen faces are unequal (caused by a much larger temperature rise at $x = 0$ than at $x = L$) and large (Biot numbers >> 1), making determination of the thermal diffusivity more difficult. For specimens in a vacuum the heat losses are by radiation, which can be described by radiation heat transfer coefficients, one on each side of the specimen. The estimation of the thermal diffusivity for tests having two heat transfer coefficients and an unknown energy input is discussed. A method is given for the simultaneous estimation of these four parameters. (Actually it is more convenient to estimate the thermal diffusivity, energy input divided by the volumetric heat capacity multiplied by the thickness, and two Biot numbers which are proportional to the heat transfer coefficients.)

Tikhonov regularization is needed in a sum of squares function to find the four parameters. The sum of squares function is minimized with respect to the parameters. Tikhonov regularization is needed because the two heat transfer coefficients are highly correlated. Methods for determining the regularization constant are discussed.

A physical understanding of the estimation problem can be obtained by examining the sensitivity coefficients for each of the parameters. The sensitivity coefficients are the first derivatives of the calculated temperature; a modified coefficient is a derivative multiplied by the appropriate parameter. If these modified coefficients are proportional over time or one is small compared to the others, the simultaneous estimation of all the parameters is very difficult because the minimum is poorly defined. However, if either of these conditions are true, the number of parameters being estimated can be reduced. Plots of the sensitivity coefficients show that the two Biot numbers are highly correlated, indicating that estimating a single Biot number is satisfactory and will not greatly affect the estimates of the thermal diffusivity. The values of Biot numbers are not important since they are nuisance parameters.

For elevated temperatures (> 1500°C), not only are the Biot numbers for the two faces highly correlated but the input energy and the Biot numbers are correlated. Thus if a reasonable estimate of the Biot number is available, only two parameters can be simultaneously estimated, namely, the thermal diffusivity and the input energy.

Several additional concepts are helpful. For oscillatory measurement errors, filtering of the data can improve the estimates. Sequential estimation (for adding one measurement after another) can yield much insight into the adequacy of the model. It is important to examine the residuals. For the experimental data examined, which is for CBCF at 2000°C, the residuals are shown to be relatively small, indicating that the model is satisfactory. Confidence regions for the measurements are given which are about ±5% for the data considered.

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