A NEW APPROACH TO THE ANALYSIS OF THERMOPHYSICAL PARAMETERS MEASUREMENT UNCERTAINTY

Svetozár Malinarič, Alžbeta Vážanová

Department of Physics, Faculty of Natural Sciences, Constantine the Philosopher University, Tr. A. Hlinku 1, SK-949 74 Nitra, Slovakia Email: smalinaric@ukf.sk, bvazanova@ukf.sk

Abstract

This work reports on thermophysical parameters (thermal conductivity and diffusivity) measurement. The influence of temperature measurement uncertainty on the parameter estimation uncertainty is studied using least squares procedure. The standard and difference analysis are used for optimizing the experiment with respect to data window. The analysis is applied to the Extended dynamic plane source method and the results of numerical computation are illustrated in the form of a contour plot.

Key words: uncertainty, least squares fitting, thermal diffusivity, thermal conductivity, difference analysis

1 Introduction

Dynamic methods [1] of measuring thermophysical parameters of solids represent a large group of techniques which use a dynamic temperature field inside the specimen. The dynamic methods can be characterized as follows. The temperature of the specimen is stabilized and uniform. Then the dynamic heat flow in the form of a pulse or step-wise function is applied to the specimen. The thermophysical parameters of the material can be calculated from the temperature response.

The measuring procedure consists of theory and experiment. The theoretical model of the experiment is described by the partial differential equation for the heat transport. The temperature function is a solution of this equation with boundary and initial conditions corresponding to the experimental arrangement. The experiment consists in measuring the temperature response and fitting the temperature function over the experimental points. Using the least squares procedure following thermophysical parameters can be estimated: thermal diffusivity a, thermal conductivity λ and specific heat capacity c.

The reliability of the measurement can be quantified by estimating its uncertainty [2]. The sources of uncertainty in dynamic methods can be divided into two groups. The first group represent the uncertainties caused by the deviations between the mathematical model and real experimental set up. The second group is created by uncertainties of input parameter measurements and evaluation method.

The aim of this work is to analyze the influence of the temperature measurement uncertainty on the thermophysical parameter estimation uncertainty. All other input parameters will be regarded as constants with zero uncertainty. Presented analysis will be applied to the Extended dynamic plane source (EDPS) method [3].

2 Uncertainty assessment in the least squares procedure

As mentioned above the first step of evaluation is to determine the temperature function - temperature increase as a function of time. Assume the function is of known analytic form

$$T(t,\vec{\alpha}) = T(t,\alpha_1,\alpha_2,\dots\alpha_p) \tag{1}$$

where t is the variable and $\vec{\alpha}$ is the vector of unknown parameters [4]. In addition to one or two thermophysical parameters, there are usually some nuisance parameters [5] connected with the model. We suppose that the deviation between model and experiment is negligible and the only source of uncertainty, in this analysis, stems from temperature measuring accuracy. We also assume that the uncertainties of temperature measurement of all points are the same and uncertainties of time measurement are negligible. As the temperature function (1) is nonlinear in parameters we have to expand it using Taylor series [6]. Then we can write the linear least squares procedure in matrix notation

$$\vec{Y} - T(\vec{t}, \vec{a}) = \mathbf{X} \cdot (\vec{\alpha} - \vec{a}) + \vec{\epsilon}$$
⁽²⁾

where \vec{Y} is the observation vector of temperature measured at n points determined by \vec{t} vector of times. $\vec{\epsilon}$ is the vector of errors, \vec{a} is the close guess for parameter vector $\vec{\alpha}$ and **X** is the sensitivity matrix [4] given by

$$\{\mathbf{X}\}_{ij} = \frac{\partial \Gamma(t_i, \vec{\alpha})}{\partial \alpha_j} = \beta_j(t_i, \vec{\alpha}) .$$
(3)

where β_j is the sensitivity coefficient for parameter α_j . Then the standard uncertainty of the least square estimate of the parameter α_j becomes

$$u^{2}(\boldsymbol{\alpha}_{j}) = \left\{ \left(\mathbf{X}^{T} \cdot \mathbf{X} \right)^{-1} \right\}_{jj} u^{2}(T) = \left(A_{j} u(T) \right)^{2}$$

$$\tag{4}$$

where u(T) is the standard uncertainty of temperature measurement. According to the equation (4) the parameter estimation uncertainty consists of two parts. The first part, designated as the coefficient A_j , is given by temperature function and selection of measured points. The second is given by temperature measurement uncertainty.

3 Standard and difference analysis

In this section we will focus on optimizing the experiment with respect to data window defined by the time interval $(t_B, t_B + t_S)$, where t_B is the beginning and t_S the size of the interval, as shown in Fig. 1. The standard and difference analysis [7] are methods of determining the time window in which the fitting procedure should be applied to obtain reliable values of thermophysical parameters. The standard analysis is based on estimating parameters using least squares procedure when t_B is kept constant while t_S is successively increased. The results of fitting are plotted against t_S . In difference analysis t_B is the variable and t_S is the constant and the results of fitting are plotted against t_B . If the time interval $(t_B, t_B + t_S)$ is not suitable for parameter estimation, the results of fitting are erroneous and the plot is scattered.



Fig 1 Temperature function and data window definition

Both methods can be applied to data from real measurements where all types of uncertainties are included. They can also be used in experiment modeling where the only source of uncertainty is simulated as random noise of temperature measurement. The third application consists in plotting the time dependence of coefficient A_j . As seen from the equation (4), low value of A_j predicts also low value of parameter estimate uncertainty $u(\alpha_j)$ and thus low scattering of parameter α_i least square estimates.

4 Dimensionless quantities

Dimensionless quantities [8] enable to perform universal numerical calculations with arbitrary specimen dimensions and thermophysical properties. Dimensionless time is defined by

$$t^{+} = \frac{a \cdot t}{l} \tag{5}$$

where a is the thermal diffusivity and l is the characteristic dimension of the specimen. Dimensionless temperature is defined by the following form

$$T^{+} = \frac{T}{T_{\rm m}} \tag{6}$$

where T_m is the maximum value of temperature function in the measuring time interval. Similarly, we can define dimensionless sensitivity coefficients

$$\beta_{j}^{+}(t,\vec{\alpha}) = \frac{\alpha_{j}}{T_{\rm m}} \frac{\partial T(t,\vec{\alpha})}{\partial \alpha_{j}}.$$
(7)

and also dimensionless coefficient A_j^+ using the equation (4) as

$$u^{+}(\alpha_{j}) = \frac{u(\alpha_{j})}{\alpha_{j}} = \frac{A_{j} \cdot T_{m}}{\alpha_{j}} \cdot \frac{u(T)}{T_{m}} = A_{j}^{+} \cdot u^{+}(T)$$
(8)

where u^+ is the dimensionless (relative standard) uncertainty [2].

5 Extended dynamic plane source method

This method is characterized by step-wise heating and one-dimensional heat flow into a finite specimen [3]. The experimental arrangement is obvious from Fig. 2. The nickel disc simultaneously serves as the heat source and thermometer. The heat is produced by the passage of an electrical current through the disc.



Fig 2 The setup of the experiment.

Two identical specimens of cylindrical shape cause symmetrical division of the heat flow into a very good heat conducting material (heat sink), which provides isothermal boundary condition of the experiment. The instantaneous value of the disc temperature is determined by measuring its resistance. The theoretical temperature function is given by the following form

$$T(t,a,\lambda,\tau) = \frac{q}{\lambda} \sqrt{\frac{ta}{\pi}} \left(1 + 2\sqrt{\pi} \sum_{n=1}^{\infty} \beta^n \operatorname{ierfc}\left(\frac{nl}{\sqrt{at}}\right) \right) + \tau$$
(9)

where q is the heat current density, l is the thickness, λ is the thermal conductivity and a is the thermal diffusivity of the specimen. Nuisance parameter τ is the base line referred to the additional increase in the temperature of the disc due to its imperfections, ierfc is the error function integral [9] and β describes the heat sink imperfection. The maximum value of the temperature function is given by

$$T_m = \frac{q \cdot l}{2 \cdot \lambda} \tag{10}$$

6 Results and discussion

Fig. 3 shows the temperature function and sensitivity coefficients as a function of time in dimensionless scale. The sensitivity coefficient is a measure of the change in temperature function due to the variation of the estimated parameter. The sensitivity coefficients analysis is based on the assumption that the fitting procedure does not work properly when sensitivity coefficients are small or linearly dependent on each other [4]. But it is very uneasy to determine the optimal time interval, in which the fitting procedure should be applied, directly form Fig. 3. Some methods for quantification of linear dependence were elaborated. In [10] the linear dependence was quantified using local curvature of the line when one sensitivity coefficient is plotted against the other. In [11] the linear dependence was investigated by the use of the Wronskian. In both methods the time interval was determined where the sensitivity coefficients were not linearly dependent. But there is no evidence of a minimum of the computed parameters uncertainty in this interval.



Fig 3 Dimensionless temperature function and dimensionless sensitivity coefficients β_a^+ and β_λ^+ vs. dimensionless time in EDPS method.



Fig 4 Contour plot of dimensionless coefficient A_a^+ as a function of dimensionless times t_s^+ and t_B^+ .



Fig 5 Contour plot of dimensionless coefficient A_{λ}^+ as a function of dimensionless times t_s^+ and t_B^+ .

The problem will be solved by means of computing the parameter estimate uncertainty for all possible time intervals using formula (8). This represents an integration of the standard and difference analysis described in section 3. Because the temperature measurement uncertainty u(T) is assumed to be constant, it proves to be useful to investigate only the coefficients A_a^+ and A_{λ}^{+} associated with the thermophysical parameters a and λ . Fig. 4 shows the dimensionless coefficient A_a^+ as a function of two variables t_s^+ and t_B^+ in the form of a contour plot, which directly enables to determine the expected uncertainty of parameter estimate for given time interval. Alternatively, we can easily find the time interval for required measurement uncertainty. In Fig. 4 we see that there is no local minimum and the coefficient is decreasing with the size of the interval. The theoretical temperature function (9) describes the real experiment only in specific time interval in which the least squares procedure can be applied. The borders of such an interval can be plotted as straight lines in Fig. 4. For example, the hatched surface represents all possible intervals, points $[t_s^+, t_b^+]$, which are subset of an interval (0.5; 2). Similarly, Fig. 5 shows the contour plot of the dimensionless coefficient A_{λ}^+ . The contour lines shows the "valley" along the straight line p with points A, B and C. This is the region where low values of uncertainty can be expected.

Fig. 6 and 7 show the dependences of dimensionless coefficient A_a^+ and A_λ^+ on dimensionless time t_B^+ for 3 values of $t_s^+ = 0$, 0.3 and 1, respectively. These plots represent the difference analysis described in section 3. Points A, B and C are situated in minimums of curves in Fig. 7 and were selected to uncertainty evaluation in Tab. 1.

The application of presented analysis was demonstrated simulating the measurement of PMMA (polymethylmetacrylate). The following values were used: l = 0.003 m, q = 500W·m⁻², $a = 0.12 \cdot 10^{-6}$ m²·s⁻¹, $\lambda = 0.19$ W·m⁻¹·K⁻¹, $\tau = 0.2$ K and $\beta = -0.954$. The sample period was 1 s and the temperature measurement uncertainty u(T) = 0.01 K. Tab. 1 shows the uncertainty evaluation for three time intervals. Using equation (5) the dimensionless times were transformed into real time windows. The dimensionless coefficients were determined by the use of Fig. 6 and 7. The relative standard uncertainties of thermophysical parameters a and λ estimates were obtained by using equations (8) and (10).



Fig 6 Values of dimensionless coefficient A_a^+ vs. dimensionless time t_B^+ (difference analysis).



Fig 7 Values of dimensionless coefficient A_{λ}^{+} vs. dimensionless time t_{B}^{+} (difference analysis).

The sharp minimum in Fig. 7 point C predicts that the optimal time interval would have non zero beginning. This is in agreement with the results in works [10-12] where the window, in which the fitting procedure should be applied, was determined approximately to $t_B^+ = 0.1$ and $t_S^+ = 1$. But current analysis proved that the curve $t_S^+ = 1$ in Fig. 6 and 7 acquired the minimum at $t_B^+ = 0$ (point A). Hence, from theoretical point of view, there is no reason for omitting data at the beginning of the time series. However, in real experiment the imperfection of the disc can cause the beginning of the measured temperature function to be destroyed as discussed in [10].

point	t^+_B	t_S^+	$t_B[s]$	$t_{s}[s]$	window [s]	A_a^+	A^+_λ	$u^{+}(a)[\%]$	$u^+(\lambda)[\%]$
А	0	1	0	75	(0; 75)	2.4	0.61	0.64	0.16
В	0.27	0.3	20	23	(20; 43)	34	3.1	9.0	0.84
C	0.4	0.03	30	2	(30; 32)	8400	94	2300	26

Tab 1 Uncertainty evaluation for tree time intervals defined by points A, B and C in Fig. 5

7 Conclusions

The paper presents the analysis of the influence of temperature measurement uncertainty on the least squares estimate uncertainty of the thermophysical parameters. The analysis is based on numerical computing the parameter estimate uncertainty for all possible time intervals. The coefficients of uncertainty A_a^+ and A_λ^+ defined by (4) and (8) are illustrated as a function of two variables t_s^+ and t_B^+ (Fig.4, 5). The analysis was applied to the thermal conductivity and diffusivity measurement of PMMA by using EDPS method. The results are presented in Fig.6, Fig.7 and Tab.1. The analysis showed that at shorter intervals ($t_s^+=0.3$) the minimum uncertainty is obtained at non zero interval beginning but at longer intervals ($t_s^+=1$) the minimum is at $t_B^+ = 0$ (point A).

Acknowledgement

Authors wish to thank the Slovak Science Grant Agency for the financial support under the contract 1/2117/05.

References

- Kubičár Ľ and Boháč V, 1999 Proc. 24th Int. Conf. on Thermal Conductivity / 12th Int. Thermal Expansion Symp. (October 26-29, 1997) ed P S Gaal and D E Apostolescu (Lancester: Technomic) 135-149
- [2] ISO 1993 Guide to the Expression of the Uncertainty in Measurement (Geneva : ISO)
- [3] Karawacki E, Suleiman B M, ul-Hag I and Nhi B, 1992 Rev. Sci. Instrum. 63, 4390-4397
- [4] Beck J V and Arnold K J, 1977 Parameter Estimation in Engineering and Science (New York: Wiley)
- [5] Vozár L, Groboth G, 1997 *High Temp.-High Press.* **29**, 191-199
- [6] Kundracik F, 1999 Spracovanie experimentálnych dát (Bratislava, UK)
- [7] Boháč V, Gustavsson M K, Kubičár Ľ and Gustafsson S E, 2000 *Rev. Sci. Instrum.* **71**, 2452-2455
- [8] Taktak R, Beck J V and Scott E P, 1993 Int. J. Heat Mass Transf. 36, 2977-2986
- [9] Carslaw H S and Jaeger J C, 1959 Conduction of Heat in Solids (Oxford: Clarendon)
- [10] Malinarič S, 2004 Meas. Sci. Technol. 15, 807-813
- [11] Malinarič S, 2004 Int. J. Thermophys. 25 1913-1919
- [12] Malinarič S, 2005 Acta Phys. Slovaca 55 165-171