A dynamic thermal identification method applied to conductor and nonconductor materials

VALÉRIO L. BORGES, SANDRO M. M. DE LIMA E SILVA and GILMAR GUIMARÃES*

School of Mechanical Engineering, FEMEC/UFU, Federal University of Uberlândia, UFU Uberlândia, MG, Brazil

(Received 10 January 2005; revised 8 April 2005; in final form 20 April 2005)

A method for determining simultaneously the thermal diffusivity, \( \alpha \), and the thermal conductivity, \( \lambda \), of conductor and nonconductor materials is presented. The precise knowledge of these properties is especially important in heat transfer problems such as heat generation, cooling behavior in machining processes, or in developing of new materials. Additional difficulties can appear in the determination of \( \alpha \) and \( \lambda \) of conductor materials. Problems of low sensitivity due to the small temperature gradient, heat loss in one-dimensional (1D) experiments, and thermal contact resistance can be cited. In this sense, a transient three-dimensional (3D) thermal model is developed. A minimization of an objective function based on the square difference between experimental and numerical phase angle in the frequency domain is used to determine \( \alpha \). Another objective function, a least square error function of measured and calculated temperatures, is used to obtain \( \lambda \). One novelty of this technique is the use of a 3D thermal model that allows the optimizing of the experimental apparatus choosing optimal sensor locations. Three different materials are investigated in this work: a AISI304 stainless steel sample and two samples of polymers (polythene and polyvinyl chloride (PVC)). The estimation results for both conductor and nonconductor sample have shown good agreement with literature.

Keywords: Thermal diffusivity; Thermal conductivity; Parameter estimation; Experimental technique

1. Introduction

Several researchers have been working on the simultaneous determination of thermal diffusivity (\( \alpha \)) and thermal conductivity (\( \lambda \)) [1–6]. However, the methods proposed in most of these works can only be used to obtain \( \alpha \) and \( \lambda \) of nonconductor materials. Additional problems appear in presence of conductive materials. Problems such as contact resistance, low sensitivity due to the small temperature gradient, and the heat flux losses are responsible for the difficulty of direct application of these methods.

*Corresponding author. Email: gguima@mecanica.ufu.br
As in any experimental method, the identification of thermal properties is sensitive to measurement uncertainty. Thus, to guarantee accuracy in the estimation, the design of the experiments should be optimized. The optimization design is related to the boundary conditions and sensor locations [6]. Beck and Arnold [6] have shown that the best experiment corresponds to a finite body with a heat flux that produces a temperature change in a surface keeping isolated the other surfaces. This basic idea for the thermal model is used here. However, to avoid the low sensitivity and the thermal contact resistance problems, the sensors are disposed in different ways using the three-dimensional (3D) model.

2. Fundamentals

2.1. Dynamic and thermal equivalent system

The technique proposed here is based on the use of an input/output dynamical system (figure 1), given by the convolution integral

\[ Y(t) = \int_{0}^{\infty} h(t - \tau)X(\tau)\,d\tau \]  

or in transformed frequency plane

\[ Y(f) = H(f) \cdot X(f) \]  

where the weighting function, \( h(\tau) \), is equal to 0 for \( \tau < 0 \) when the system is physically realizable. In frequency domain, \( H(f) \) represents the frequency response which is defined as the Fourier transform of \( h(\tau) \),

\[ H(f) = \int_{0}^{\infty} h(\tau)e^{-j2\pi f\tau}\,d\tau \]  

where \( j = \sqrt{-1} \) is the imaginary unit [7].

The dynamic model can be obtained from a thermal model shown in figure 2, where \( \phi_{i} \) represents the heat flux, \( T_{i} \) the temperature and \( i \) is the index used to describe the location of the respective heat flux and the temperature in the sample.

In this thermal model the input, \( X(t) \), and output, \( Y(t) \), data are defined, respectively as: \( X(t) = \phi_{1}(t) \) and \( Y(t) = \theta_{1}(t) - \theta_{2}(t) \), where \( \theta(t) \) is defined as \( T(t) - T_{0} \).

The 3D thermal model can be obtained by the solution of the diffusion equation

\[ \frac{\partial^{2}T}{\partial x^{2}} + \frac{\partial^{2}T}{\partial y^{2}} + \frac{\partial^{2}T}{\partial z^{2}} = \frac{1}{\alpha} \frac{\partial T}{\partial t} \]  

Figure 1. Input/output dynamic system.
in the region \( R (0 < x < a, 0 < y < b, 0 < z < c) \) and \( t > 0 \), subjected to the boundary conditions:

\[
\begin{align*}
-\lambda \frac{\partial T}{\partial y} \bigg|_{y=b} &= \phi_1(t) \quad \text{at } S_1(0 \leq x \leq x_H, 0 \leq z \leq z_H) \\
-\lambda \frac{\partial T}{\partial y} \bigg|_{y=0} &= 0 \quad \text{at } S_2(x, z \in S | (x, z) \notin S_1)
\end{align*}
\tag{4b}
\]

\[
\frac{\partial T}{\partial x} \bigg|_{x=0} = \frac{\partial T}{\partial x} \bigg|_{x=a} = \frac{\partial T}{\partial y} \bigg|_{y=0} = \frac{\partial T}{\partial y} \bigg|_{y=c} = \frac{\partial T}{\partial z} \bigg|_{y=b} = 0
\tag{4c}
\]

and the initial condition

\[
T(x, y, z, 0) = T_0
\tag{4d}
\]

where \( S \) is defined by \((0 \leq x \leq a, 0 \leq z \leq c)\) and \( x_H e y_H \) are the boundary of \( S_1 \) where the heat flux is applied.

If \( T(r, t) \) represents \( T(x, y, z, t) \), the solution of equations (4) can be given in terms of Green’s function \( G \)

\[
T(r, t) - T_0 = \int_{\tau=0}^{t} \left[ \int_{y'} \frac{\alpha}{\lambda} G(r, t', t - \tau) \bigg|_{y'=b} dS' \right] \phi_1(t) d\tau
\tag{5}
\]

where the Green’s function \( G(r, t', t - \tau) = G(x, y, z/x', y', z', t - \tau) \) is available for the homogeneous version associated to the problem defined by equations (4) [8].

Although the Green’s function is available [9], it will not be used in this work. As described in a previous work [10] the solution of the problem defined by equations (4) is performed numerically. However, equation (5) reveals that an equivalent thermal
model can be associated with the dynamic model given by equation (2). In this case, using the same procedure described in the one-dimensional (1D) case in the previous work [10] the equivalent thermal model can be obtained as the convolution product in the frequency domain.

\[
\theta_1(f) - \theta_2(f) = G_{12}^+(f)\phi_1(f)
\]  

(6)

where the variable \( f \) indicates that Fourier transform was applied to the variables \( \theta, \phi, \) and \( G_{12}^+ \). A comparison of equation (6) with equation (1) gives

\[
G_{12}^+(t - \tau) = h(t - \tau) = \frac{\alpha}{\lambda} [G(x_1, y_1, z_1, t - \tau) - G(x_2, y_2, z_2, t - \tau)]
\]  

(7)

It can be observed that as \( \phi(t) \) e \( \theta(t) \) are obtained by discrete measurements, Fourier transforms can be performed numerically by using the Cooley–Tukey algorithms (Discrete Fast Fourier Transform) for these data [7]. Therefore, the equivalent thermal system to the dynamic system can be represented by:

\[
Z(f) = h(f) = \frac{\theta_1(f) - \theta_2(f)}{\phi_1(f)} = \frac{Y(f)}{X(f)}
\]  

(8)

where the function \( Z(f) \), also called impedance generalized, is equivalent to the response in frequency \( H(f) \) defined by equation (2). Observing equations (4) it can be concluded that the frequency response \( H(f) \) is strongly dependent of the thermal properties, which means:

\[
H(f) = \frac{\theta_1(f) - \theta_2(f)}{\phi_1(f)} = \text{function} (\alpha, \lambda)
\]  

(9)

It should be observed that the transformed impedance in the \( f-x \) plane is a complex variable which in a polar form can be written by

\[
Z(f) = H(f) = |H(f)| e^{j\varphi(f)}
\]  

(10)

where \( |H| \) and \( \varphi \) represent, respectively the modulus and the phase factor of \( H \). The phase factor can be written by

\[
\varphi(f) = \arctan \frac{\text{Im} H(f)}{\text{Re} H(f)}
\]  

(11)

where \( \text{Re} H(f) \) and \( \text{Im} H(f) \) are the real and imaginary parts of \( H \).

The phase of frequency response \( H(f) \) and the time evolution of superficial temperatures, \( T_1(t) \), and \( T_2(t) \) are the experimental data used for estimation of thermal diffusivity and thermal conductivity respectively.

2.2. Thermal diffusivity estimation: frequency domain

The fact that the phase factor is just a function of the thermal diffusivity \( \alpha \) is the great convenience of working in the frequency domain. The basic idea here is the observation that the delay between the experimental and theoretical temperature is an exclusive function of \( \alpha \). Therefore, the minimization of an objective function, \( S_p \), based on the
difference between experimental and calculated values of the phase is used to determine the thermal diffusivity. This function can be written as

\[ S_p = \sum_{i=1}^{N_f} (\varphi_e(i) - \varphi_t(i))^2 \]  

(12)

where \( \varphi_e \) and \( \varphi_t \) are the experimental and calculated values of the phase factor of \( H \) respectively. The theoretical values of the phase factor are obtained from the identification of \( H(f) \) by equation (11). In this case, the output \( Y(f) \) is the Fourier transform of the difference \( \theta_1(t) - \theta_2(t) \) obtained by the numerical solution of equations (4) using the finite volume method [11]. In fact, this procedure avoids the necessity of obtaining an explicit and analytical model of \( H(f) \).

The values of \( \alpha \) will be supposed to be those that minimize equation (12). In this work, this minimization is done by using the golden section method with polynomial approximation [12].

2.3. Thermal conductivity estimation: time domain

Once the thermal diffusivity value is obtained, an objective function based on least square temperature error can be used to estimate the thermal conductivity. In this case, there is no identification problem as just one variable is being estimated. Therefore, the variable \( \lambda \) will be supposed to be the parameter that minimizes the least square function, \( S_{mq} \), based on the difference between the calculated and experimental temperature defined by

\[ S_{mq} = \sum_{j=1}^{s} \sum_{i=1}^{n} [\theta_e(i,j) - \theta_t(i,j)]^2 \]  

(13)

where \( \theta_e(i,j) \) is the experimental temperature and \( \theta_t(i,j) \) is the calculated temperature, \( n \) is the total number of time measurements and \( s \) represents the number of sensors. The optimization technique used to obtain \( \lambda \) is also the golden section method with polynomial approximation [12].

3. Sensitivity analysis

Although the thermal contact resistance and the low gradient problems do not represent any difficulties for non-metallic materials, they must be taken into account in the presence of conductor materials. This section discusses both problems.

Figure 3a presents the thermal contact resistance that can appear between sample and sensors in a 1D model. Figure 3b presents the 3D alternative model to avoid this problem. Another advantage in a 3D model is the experimental flexibility allowing the optimal location of the identification sensors.

In 1D model, a high magnitude of heat flux (input) can be necessary to establish a thermal gradient high enough for the estimation process. Figures 4 and 5 present a simulation using the same heat flux input. It can be observed that, while the temperature gradient is situated in the region of the uncertainty of thermocouples
(±0.3 K) (figure 4a), the three-dimensional model produces a sufficient gradient to properties estimation (figure 4b). Figure 5 presents the difference between the two temperatures involved in each model as shown in figure 3.

This fact can be better analyzed through a sensitivity analysis. Small and/or inaccurate values of temperature difference and heat flux signals produce linear dependence or low values. The linear dependence of two or more coefficients indicates that the parameters cannot simultaneously be estimated. Low values indicate that the estimation is strongly sensitive to the measurements uncertainty [6]. The sensitivity
coefficients involved in this technique are defined as follows and presented in figures 6 and 7.

\[
S_{T,\alpha} = \frac{\alpha}{T} \frac{\partial T}{\partial \alpha}, \quad S_{T,\lambda} = \frac{\lambda}{T} \frac{\partial T}{\partial \lambda}, \quad S_{\psi,\alpha} = \frac{\alpha}{\psi} \frac{\partial \psi}{\partial \alpha}, \quad S_{\psi,\lambda} = \frac{\lambda}{\psi} \frac{\partial \psi}{\partial \lambda},
\]

\[
S_{H,\alpha} = \frac{\alpha}{|H|} \frac{\partial |H|}{\partial \alpha} \quad \text{and} \quad S_{H,\lambda} = \frac{\lambda}{|H|} \frac{\partial |H|}{\partial \lambda},
\] (14)
Figure 6 reveals a linear dependency of $S_{T,\alpha}$ and $S_{T,\lambda}$ as shown by the symmetry. This fact indicates that both thermal properties cannot be estimated simultaneously in the time domain justifying the use of frequency domain for the thermal diffusivity estimation.

The sensitivity coefficients of phase related to the thermal diffusivity and thermal conductivity for 1D and 3D model are presented in figure 7.

It can be observed in figure 7 that the values of the sensitivity of phase related to the thermal diffusivity are higher for the 3D model and there is no possibility to estimate the thermal conductivity in frequency domain due to $S_{\phi,\lambda} = 0$ for any frequency value. This fact reveals that the phase dependency with thermal diffusivity is unique and exclusive.

Another advantage of using a 3D model is the possibility of estimating thermal properties from a thin sample. In the 1D case, for conductor materials, it is very hard to obtain temperature gradients with values high enough to allow a good estimation as in figure 8. For a sample with thin thickness, it can be seen that no temperature variation in the direction $y$ is observed. This fact makes the one-dimensional analysis unpractical.
Another important characteristic of the technique presented here is the very low sensitivity of $\alpha$ related to the amplitude of the signals $X$ and $Y$. It means that the estimated value of the thermal diffusivity is insensitive to bias error, like uncertainty due to poor calibration of thermocouples or heat flux transducers or both. This fact can be demonstrated by verifying figures 9 and 10 which show the behavior of phase factor

![Figure 9. Phase factor subjected to the original and calibrated pair of input/output data.](image)

![Figure 10. Modulus of $Z$ for the original and calibrated pair input/output.](image)
and modulus due to the same input/output signals in both versions: original data, \( \mu \text{V m V}^{-1} \), and calibrated data \( \text{W m}^{-2} \, ^{\circ}\text{C} \).

It can be observed in figures 9 and 10 that there are no changes in the phase factor while the modulus is strongly affected.

4. Experimental

4.1. Conductor material application

It can be observed that the boundary conditions present in the theoretical model must be guaranteed in the experimental apparatus. It means that the isolated condition at the reminiscent surface needs to be reached for the success of the estimation techniques. A good way to reach the isolation condition in a vertical direction is the use of a symmetric experiment apparatus. Figure 11 presents this scheme.

Figure 11. Schematic of experimental apparatus.
The effect of no heat flux lateral loss is reached by placing insulating material such as expanded polystyrene as shown in figure 11. Two AISI304 stainless steel samples were used in a symmetric assembly, both with thickness of 10 mm and lateral dimensions of $139 \times 65$ mm. The sample initially in thermal equilibrium at $T_0$ is then submitted to a unidirectional and uniform heat flux. The heat is supplied by a $318\,\Omega$ electrical resistance heater, covered with silicone rubber, with lateral dimensions of $50 \times 50$ mm and thickness 0.3 mm. The heat flux are acquired by a transducer with lateral dimensions of $50 \times 50$ mm, thickness 0.5 mm, and constant time less than 10 ms. The transducer is based on the thermopile conception of multiple thermoelectric junction (made by electrolytic deposition) on a thin conductor sheet [3]. The temperatures are measured using surface thermocouples (type k). The signals of heat flux and temperatures are acquired by a data acquisition system HP Series 75 000 with voltmeter E1326B controlled by a personal computer.

Twenty independent runs were performed. In each of the experiments 1024 points were acquired, at time intervals of 0.54 s. The time duration of heating, $t_h$, was approximately 120 s with a heat pulse generated at 90 V (DC).

Figure 12 shows the evolution of the input/output normalized signals in function of time for one of the experiments of AISI304 sample.

Tables 1 and 2 present, respectively, the value estimated of $\alpha$ and $\lambda$ for the AISI304 stainless steel sample.

In table 3 a summary of the simultaneous estimation of $\alpha$ and $\lambda$ of the AISI304 sample is presented. In this table, the value obtained for $\alpha$ using the Flash method [13] and the value of $\lambda$ from Incropera and DeWitt [14] are also presented.

An excellent agreement can be observed between the values of this work and the literature for the thermal diffusivity and the thermal conductivity (error less than 2%).

![Figure 12. Input data of a typical run.](image)
These results show the potential of the method proposed here. The comparison between the experimental and estimated temperatures for $\alpha = 3.76 \times 10^{-6} \text{ m}^2 \text{ s}^{-1}$ and $\lambda = 14.64 \text{ W m K}^{-1}$ is shown in figure 13. In this figure a good agreement between the data can be observed; the residuals are situated in the range of uncertainty measurement of thermocouples, that in this work is $\pm 0.3 \text{ K}$.

<table>
<thead>
<tr>
<th>Thermal properties</th>
<th>This work</th>
<th>References [13,14]</th>
<th>Error (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\alpha \times 10^{-6} \text{ (m}^2 \text{ s}^{-1})$</td>
<td>3.762</td>
<td>3.82</td>
<td>1.54</td>
</tr>
<tr>
<td>$\lambda \text{ (W m K}^{-1})$</td>
<td>14.64</td>
<td>14.90</td>
<td>1.77</td>
</tr>
</tbody>
</table>

Table 1. Statistical data of the average value of $\alpha$ (initial value of $\alpha = 1.0 \times 10^{-6} \text{ m}^2 \text{ s}^{-1}$).

Table 2. Statistical data of the average value of $\lambda$ (initial value of $\lambda = 10 \text{ W m K}^{-1}$).

Table 3. Summary of $\alpha$ and $\lambda$ for AISI304 sample.

Figure 13. Output of a typical run.
4.2. Nonconductor material application

The thermal identification technique can also be applied to nonconductor solid materials. In this case, a one-dimensional model can be used. This section presents some results of $\alpha$ and $\lambda$ estimation for two different polymers: polythene and polyvinyl chloride (PVC). More details about the 1D model and its respective sensitivity analysis can be found in [10].

Two polymers samples were used, polythene and PVC, both with thickness of 50 mm and lateral dimensions of $305 \times 305$ mm. Figure 14 shows the experimental apparatus where at time $t=0$, the sample is in thermal equilibrium at $T_0$. At this instant, the sample is submitted to a unidirectional and uniform heat flux on its upper surface. The heat is supplied by a $22 \Omega$ electrical resistance heater, covered with silicone rubber, with lateral dimensions of $305 \times 305$ mm and thickness 1.4 mm. The heat flux and temperature are acquired using sensor and instruments with the same specification of that described here in the conductor material application.

Fifty independent runs for PVC and twenty independent runs for polythene were realized. For both samples 1024 points were taken. The time intervals, $\Delta t$, were 7.034 s for PVC and 6.243 s for polythene. The time duration of heating, $t_h$, was approximately 150 s for PVC and 90 s for polythene with a heat pulse generated at 40 V (DC) for both samples.

Tables 4 and 5 present respectively the value estimated of $\alpha$ and $\lambda$ for the fifty runs of PVC, with 99.87% confidence interval. In table 6 a summary of the simultaneous estimation of $\alpha$ and $\lambda$ of the PVC sample is presented. In this table, the comparison with the values obtained for $\alpha$ by using the Flash method [14] and $\lambda$ by using the guarded hot plate method [15] presented errors of 3.22 and 3.30% for $\alpha$ and $\lambda$, respectively.

In figure 15a a comparison between experimental and estimated phase factor is presented. A very good agreement can be observed between them. Figure 15b shows the residuals.
The comparison between the experimental and estimated temperatures for \(\alpha = 1.24 \times 10^{-7} \text{ m}^2 \text{s}^{-1}\) and \(\lambda = 0.152 \text{ W m K}^{-1}\) is shown in figure 16a. Again a good agreement between the data can be observed. It can be noted that the residuals presented in figure 16b are situated in the range of uncertainty measurement of

<table>
<thead>
<tr>
<th>(\alpha (\text{m}^2 \text{s}^{-1}) \times 10^7)</th>
<th>(\lambda (\text{W m K}^{-1}))</th>
<th>Initial (S_{mq} \times 10^{-6})</th>
<th>Final (S_{mq})</th>
<th>(\sigma \times 10^7 (\text{W m K}^{-1}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.24 (\pm) 1.88%</td>
<td>0.152</td>
<td>1.351</td>
<td>5.91</td>
<td>4.9</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>(\alpha (\text{m}^2 \text{s}^{-1}) \times 10^7)</th>
<th>(\alpha (\text{m}^2 \text{s}^{-1}) \times 10^7 (\text{FM}))</th>
<th>(\lambda (\text{W m K}^{-1}))</th>
<th>(\lambda (\text{W m K}^{-1})) (HPM)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.24 (\pm) 1.88%</td>
<td>1.28 (\pm) 3.1%</td>
<td>0.152 (\pm) 1.1%</td>
<td>0.157</td>
</tr>
</tbody>
</table>

Figure 15. Phase factor: (a) experimental and calculated data (b) residuals.
thermocouples, that in this work is ±0.3 K. Table 7 presents a summary of the simultaneous estimation of $\alpha$ and $\lambda$ for the polythene sample with a confidence interval of 99.87%. For this sample only the reference value for $\lambda$ obtained by NPL [15] is presented.

5. Conclusion

In this work we have proposed a technique to simultaneously estimate the thermal diffusivity and the thermal conductivity. The technique can be used in both conductor and nonconductor solids. Two polymers and an AISI304 sample are used. The results have shown good agreement when compared with literature values for all
samples tested. The calculation of the phase factor numerically is one of the important advantages of the technique proposed here. This procedure allows the use of a 3D transient model and consequently its application to conductor material identification. The estimation of thermophysical properties of complex forms (such as a cutting tool) is a subject for future study.

**Nomenclature**

- \( f \) = frequency (Hz)
- \( G \) = Green’s function (m\(^2\) K W\(^{-1}\))
- \( H(f) \) = frequency response function (m\(^2\) K W\(^{-1}\))
- \(|H(f)|\) = modulus of frequency response function
- \( \text{Im}(S_{xy}) \) = imaginary component of the cross-spectral density function (K\(^2\))
- \( \text{Re}(S_{xy}) \) = real component of the cross-spectral density function (K\(^2\))
- \( S_{mq} \) = objective function (K\(^2\))
- \( S_{\phi} \) = phase objective function (rad\(^2\))
- \( S_{xx} \) = autoespectral density function of \( x(t) \) (K\(^2\))
- \( S_{yy} \) = autoespectral density function of \( y(t) \) (K\(^2\))
- \( S_{xy} \) = cross-spectral density function (K\(^2\))
- \( t \) = time (s)
- \( T_0 \) = initial temperature (°C)
- \( X(t) \) = input signal in time domain (°C)
- \( Y(t) \) = output signal in time domain (°C)
- \( X(f) \) = input signal in frequency domain (°C)
- \( Y(f) \) = output signal in frequency domain (°C)
- \( x, y, z \) = geometric variables (m)
- \( Z \) = generalized impedance (m\(^2\) K W\(^{-1}\))

**Greek symbols**

- \( \alpha \) = thermal diffusivity (m\(^2\) s\(^{-1}\))
- \( \lambda \) = thermal conductivity (W m K\(^{-1}\))
- \( \phi \) = heat flux (W m\(^{-2}\))
- \( \rho \) = density (kg m\(^{-3}\))
- \( \theta \) = temperature difference (°C)
- \( \psi(f) \) = phase angle (rad)

**Subscripts**

- \( t \) = relative to calculated data
- \( e \) = relative to experimental data
\[ m = \text{relative to integer variables} \]
\[ 1 = \text{relative to the thermocouple 1} \]
\[ 2 = \text{relative to the thermocouple 2}. \]

**Acknowledgements**

The authors thanks CAPES, Fapemig and CNPq.

**References**


