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Thermal conductivity estimation in non-linear problems

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Abstract

This paper reports on the development of a new application of the thermal probe in the determination of the thermal conductivity in non-linear problems. The method uses a direct non-linear numerical model associated with a parameter estimation technique to determine temperature dependent conductivities. Using enthalpy as the primary variable in the numerical model, phase change situations can easily be accommodated. The potential and effectiveness of the method are shown through test data obtained by simulated experiments.

Keywords: Thermal conductivity; Parameter estimation; Non-linear; Phase change; Numerical

1. Introduction

During these last decades the development of the technology has lead to an increasing effort in the determination of material properties. Amongst these properties the thermal conductivity is an important parameter in heat transfer and is fundamental in accurately modelling and simulating physical problems. Several techniques have been developed for the measurement of the thermal conductivity but most of them were restricted to linear cases where the conductivity is independent of other parameters like temperature. One of the most used methods is the thermal probe with its two major advantages: it is based on a transient mathematical model which makes it fast (as opposed to steady-state techniques, e.g. the Hot Box) and is compact and transportable (i.e. can be used for in situ measurements). The theory behind the thermal probe is based on the hot wire technique developed by Van Der Held and Van Drunen [1] and Blackwell [2]. A known heat flux Q is dissipated during a certain time in the cylindrical probe and the corresponding temperature rise in the probe is measured. This temperature variation depends, among other parameters, on the thermal conductivity k of the sample, see Fig. 1.

The solution of the governing heat conduction differential equation in cylindrical co-ordinates leads to an expression of the probe temperature rise in the form: $\Delta T(t) = \frac{Q}{4\pi k}\ln t + \frac{Q}{4\pi k}\left(\ln\frac{4a}{r_i^2} - \gamma + \frac{2k}{r_i R_i}\right)$, where r_i is the probe radius, R_i is the thermal resistance at the probe-sample interface and γ is Euler constant. The graph of the function $\Delta T(t) = f(\ln t)$ is linear and k is determined from the slope $Q/4\pi k$.

Due to its simplicity and ease of use this method found a wide spectrum of applications ranging from ceramics and soils to fluids and concentrated chemical solutions [3–7].

However, due to their complexity, non-linear problems (including phase change) are very difficult, if not impossible in most cases, to deal with through analytical mathematical treatment. They have then rarely been addressed and there is a lack of data on thermophysical properties in non-linear temperature intervals. Some studies used linear techniques over small temperature intervals where the thermophysical properties are assumed constant to cover the entire non-linear range [8–10], but this is time consuming and in highly non-linear problems, the necessity of considering very small temperature intervals inevitably leads to sources of

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Nomenclature

a	diffusivity
c_p	specific heat
g	heat generation rate
H	enthalpy
h	convective coefficient
k	thermal conductivity
p	number of parameters
Q	heat flux
R	thermal resistance
r	radius
T	temperature
t	time
X	sensitivity coefficient
Y	measured temperature

Greek symbols

β	parameter to be estimated
ε	measurement error
ρ	density
$\mathbf{\Omega}$	stabilising matrix

Subscripts

i	index for time or node
j	index for estimated parameters

Superscripts

n, k	iteration indices

experimental errors [11]. An analytical analysis based on Stefan and Neumann theory has been carried out but was limited to pure materials where phase change occurs at a single constant temperature [12].

At the same time, with the increasing use of simulation codes in industry and research, demand for accurate values of thermal conductivity and other material parameters is growing. For example in the food industry, where frozen goods are increasingly consumed, temperature dependent thermal conductivity values are often obtained through linear interpolation which can lead to errors in case of high non-linearity [13]. Another example lies in building energy savings where phase change materials are seen to be one of the most important ways in cutting CO_2 emission through solar or recycled energy storage [14]. Parameter estimation techniques can provide a solution to these problems. They are based on the minimisation of a quadratic criterion representing the difference between measured variations of physical quantities (usually the temperature) and the corresponding calculated ones through a mathematical model. Their clear benefit resides in the fact that the mathematical model does not have to be analytical as an explicit formulation of the measured parameter is not needed. In fact, associated with numerical modelling in complex physical problems (e.g. non-linear) parameter estimation techniques can prove to be an indispensable tool [15].

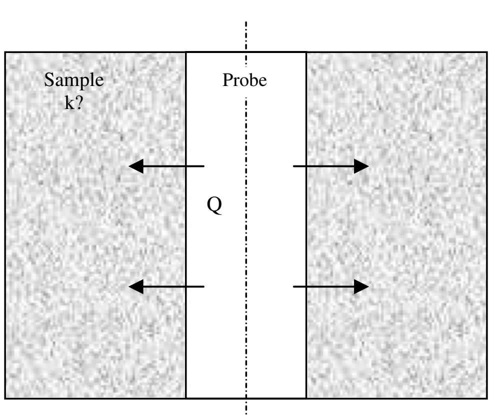

Fig. 1. Thermal probe principle.

In this study an attempt is made to bring together the advantages of the thermal probe as an experimental set-up (i.e. ease of use, in situ measurement, etc.) and the power of parameter estimation techniques in the determination of the thermal conductivity in non-linear problems. As a first phase of this research programme, the feasibility and limits of the suggested new method are evaluated through numerical simulations using computer generated temperatures. The second phase dealing with the experimental work and application of this method to a phase change problem will be the object of a following paper in due course.

The principle of the thermal probe is maintained, see Fig. 1, the novel part is the mathematical treatment of the temperature rise in the probe ($\Delta T = f(\text{time})$) using a parameter estimation technique. Practically, the temperature rise will be measured using a single thermocouple in the glue layer of the probe. For a constant power supply Q over a certain time, ΔT provides a signal used in the determination of the evolution of the thermal conductivity with the temperature at a set number of points.

2. Numerical model

The system to be modelled is a cylindrical multi-layer arrangement: the sample and the probe with its three components (the hot wire, the glue maintaining it and the external tube), see Fig. 2. The non-linear cylindrical governing equation is:

$$\frac{1}{r}\frac{\partial}{\partial r}\left(k(r,T)r\frac{\partial T}{\partial r}\right) + g(r) = \rho(r,T)c_p(r,T)\frac{\partial T}{\partial t} \quad (1)$$

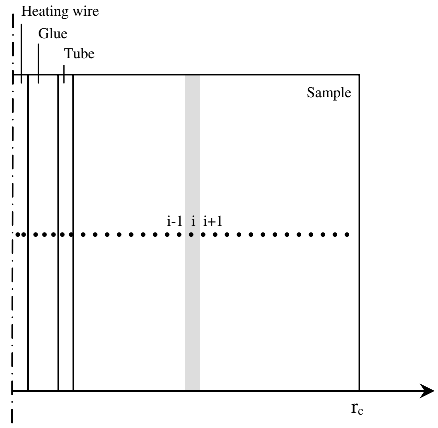

Fig. 2. Subdivision of the system (not to scale).

with the initial condition $t = 0, \quad T(r) = T_0 \;\; 0 \leqslant r \leqslant r_c,$
the boundary conditions $r = 0, \quad k(T)\frac{\partial T}{\partial r} = 0,$
$r = r_c, \quad -k(r,T)\frac{\partial T}{\partial r} = h(T(r_c) - T_0),$

where ρ is the density, c_p is the specific heat, g the heat generation term and h the convective heat transfer coefficient. This model does not take into account convective effects in the liquid phase as it is purely used to demonstrate the potential of the method through computer simulations.

In order to be able to treat phase change problems without dealing with the solid/liquid interface, Eq. (1) is rewritten using enthalpy H (which includes the latent heat) as variable. It is assumed that enthalpy is a piecewise linear function of temperature ($T = AH + B$):

$$\frac{1}{r}\frac{\partial}{\partial r}\left(k(r,H)r\frac{\partial(AH+B)}{\partial r}\right) + g(r) = \rho(r,H)\frac{\partial H}{\partial t}. \tag{2}$$

A numerical solution to Eq. (2) is obtained using an energy balance technique [21]. For node i, the heat balance can be written as

$$2\pi r_i \Delta r \rho_i \frac{\mathrm{d}H_i}{\mathrm{d}t} = \frac{(AH+B)_{i+1} - (AH+B)_i}{[1/(2\pi k_{i,i+1})]\ln(r_{i+1}/r_i)} + \frac{(AH+B)_{i-1} - (AH+B)_i}{[1/(2\pi k_{i-1,i})]\ln(r_i/r_{i-1})} + g_i. \tag{3}$$

With an implicit numerical scheme, Eq. (3) becomes:

$$\begin{aligned}&\left(2\pi r_i \Delta r \rho_i \frac{\Delta t A_i}{[1/(2\pi k_{i,i+1})]\ln(r_{i+1}/r_i)} + \frac{\Delta t A_i}{[1/(2\pi k_{i-1,i})]\ln(r_i/r_{i-1})}\right)H_i^{n+1}\\ &\quad + \left(-\frac{\Delta t A_{i+1}}{[1/(2\pi k_{i,i+1})]\ln(r_{i+1}/r_i)}\right)H_{i+1}^{n+1}\\ &\quad + \left(-\frac{\Delta t A_{i+1}}{[1/(2\pi k_{i-1,i})]\ln(r_i/r_{i-1})}\right)H_{i-1}^{n+1}\\ &\quad = (2r_i \Delta r \rho_i)H_i^n + \frac{\Delta t(B_{i+1} - B_i)}{[1/(2\pi k_{i,i+1})]\ln(r_{i+1}/r_i)}\\ &\qquad + \frac{\Delta t(B_i - B_{i-1})}{[1/(2\pi k_{i-1,i})]\ln(r_i/r_{i-1})} + g_i \Delta t\end{aligned} \tag{4}$$

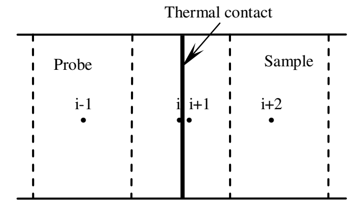

Fig. 3. Probe-sample interface.

In order to avoid using an average thermal conductivity between the probe and the sample, the thermal contact between these two materials is treated through half volumes either side of the interface. The corresponding nodes exchange heat energy through the thermal resistance only, see Fig. 3.

Linear equations can be written for all nodes and a matrix formulation is used as follows:

$$\mathbf{A}^{n+1}\mathbf{H}^{n+1} = \mathbf{B}^{n+1}, \tag{5}$$

where **A** is the coefficient matrix, **H** is the vector of the unknown enthalpies, and **B** is the known coefficient vector whose elements involve contributions due to energy generation and boundary conditions for the problem.

The computer program developed uses a variable time step scheme. Typical initial time step of 1 s is reduced progressively according to preset criteria (i.e. convergence, maximum number of iterations) during the phase change. After the phase change when convergence is quicker the time step is progressively increased back to the initial value. Similarly, the space grid resolution is finer in and immediately around the probe to take account of the localised phase change heat transfer. A total number of nodes of 800 was necessary to allow convergence for phase change occurring at small temperature interval (where the slope of the line $\mathbf{AH} + \mathbf{B}$ is very steep).

At each time step n, Gauss elimination method is used to solve:

$$\mathbf{H} = \mathbf{A}^{-1}\mathbf{B}. \tag{6}$$

This model has been validated against an available exact solution for a non-linear heat sink problem [16] and an experimental linear measurement [17].

3. Parameter estimation method

A sample is subjected to a heat flux and the temperature rise in the probe is measured. This output signal is a function of the input heat flux and the unknown conductivity of the sample.

$\boldsymbol{\beta}$ denotes the parameter vector to be estimated (conductivities), the maximum number of parameters p that can be estimated is determined through a sensitivity study (see Section 4):

$$\boldsymbol{\beta} = (\beta_1, \beta_2, \ldots, \beta_p). \tag{7}$$

The least square function S to be minimized is:

$$S(\boldsymbol{\beta}) = \sum_{i=1}^{n} (Y(t_i) - T(t_i, \boldsymbol{\beta}))^2, \tag{8}$$

where $Y(t_i)$ represents the measured temperature in the probe at time t_i ($1 \leqslant i \leqslant n$) and $T(t_i, \boldsymbol{\beta})$ is the corresponding calculated temperature at the same time. In this paper $\mathbf{T}(t, \boldsymbol{\beta})$ is obtained from the numerical model. When the mathematical model is accurate it can be assumed that $\mathbf{Y}(t) = \mathbf{T}(t, \boldsymbol{\beta}) + \boldsymbol{\varepsilon}(t)$ where $\boldsymbol{\varepsilon}$ is the measurement and numerical approximation error.

The minimum of $S(\boldsymbol{\beta})$ occurs when:

$$\frac{\partial S(\boldsymbol{\beta})}{\partial \beta_j} = -2 \sum_{i=1}^{n} [(Y(t_i) - T(t_i, \boldsymbol{\beta}))] X_j(t_i, \boldsymbol{\beta}) = 0, \tag{9}$$

where $1 \leqslant j \leqslant p$ and $X_j(t_i, \boldsymbol{\beta}) = \partial T(t_i, \boldsymbol{\beta}) / \partial \beta_j$ is the sensitivity coefficient. It expresses the change of the temperature due to a change in the parameter β_j. Only parameters with uncorrelated (not linear dependent) sensitivity coefficients can be estimated [15]. When the mathematical model is numerical, as in this case, coefficients X_j can be calculated using finite differences. At each iteration, and based on the previous value of β_j, X_j can be expressed as

$$X_j = \frac{T(t, \beta_1, \ldots, \beta_j + \delta\beta_j, \ldots, \beta_p) - T(t, \beta_1, \ldots, \beta_j - \delta\beta_j, \ldots, \beta_p)}{\delta\beta_j}, \tag{10}$$

where δ is a small number usually taken between 10^{-5} and 10^{-2} [15]. If computing time is a limiting factor, backward or forward difference approximation can also be used.

Eq. (9) may be rewritten in a matrix format:

$$\mathbf{X}^{\mathrm{T}}(\boldsymbol{\beta})[\mathbf{Y} - \mathbf{T}(\boldsymbol{\beta})] = 0. \tag{11}$$

Assuming a linear dependence on the parameters β_j (i.e. $\mathbf{T} = \mathbf{X}\boldsymbol{\beta}$) the solution for $\boldsymbol{\beta}$ is:

$$\boldsymbol{\beta}(\mathbf{X}^{\mathrm{T}}\mathbf{X})^{-1}\mathbf{X}^{\mathrm{T}}\mathbf{Y}. \tag{12}$$

When the problem is non-linear, as it is the case here, it must be treated in an iterative manner:

$$\boldsymbol{\beta}^{(k+1)} = \boldsymbol{\beta}^{(k)} + [\mathbf{X}^{\mathrm{T}}\mathbf{X}]^{-1}[\mathbf{X}^{\mathrm{T}}(\mathbf{Y} - \mathbf{T}(\boldsymbol{\beta}^{(k)}))]. \tag{13}$$

The iterations are continued until negligible variation occurs between $\boldsymbol{\beta}^{(k+1)}$ and $\boldsymbol{\beta}^{(k)}$.

4. Sensitivity study

In order to determine the optimal experimental configuration (heating time, heat flux intensity, etc.) a study of the system sensitivity to different parameters influencing the temperature rise is performed. The case simulated here includes a phase change for the material water–agar (4% in mass). The enthalpy variation with temperature over a range of 15 °C is shown in Fig. 4 [19]. The phase change occurs between approximately −2 °C and 0 °C where the enthalpy increases sharply by a value corresponding to the latent heat.

The unknown thermal conductivity is determined at a certain number of pre-defined temperatures with the assumption of linear variation between each two points. For each simulation these pre-defined temperatures can be changed in the model to cover as finely as possible the entire temperature range of interest. The model response is the temperature variation in the probe.

Taking an initial temperature of −8 °C and a heating power of 40 W/m over a duration of 100 s, the sensitivity of the model to the thermal conductivity of the tested material at seven different temperatures appears in Fig. 5. Note that in order to easily visualise the effect of each parameter, reduced sensitivity coefficients $\frac{\partial T(t_i, \boldsymbol{\beta})}{\partial \beta_j} \beta_j$ have been used here to provide the absolute temperature variation due to a relative variation of β_j.

Several key points can be highlighted from the graph:

- The model becomes sensitive to k (2 °C) towards the end of the heating time when the sample reaches and goes beyond that temperature. Similarly, the sensitivity to k (4 °C) is nil which implies that this parameter is certainly impossible to estimate (the sample not reaching that temperature).
- The sensitivity to the conductivity at the initial temperature, k (−8 °C), is relatively low as the temperature of the sample around the probe increases rapidly away

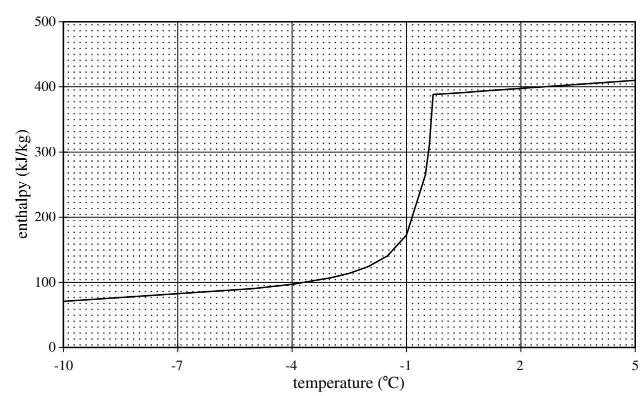

Fig. 4. Enthalpy versus temperature for the gel water–agar.

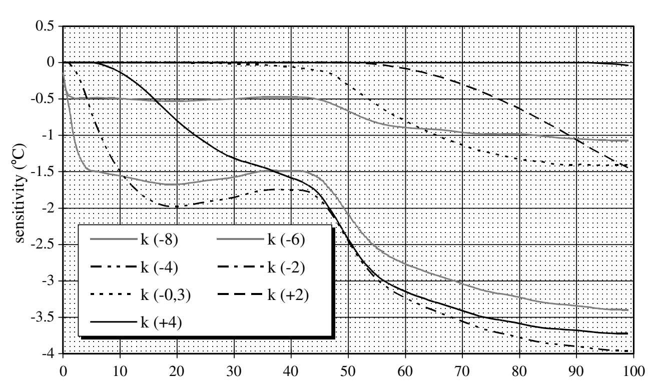

Fig. 5. Sensitivity to thermal conductivities.

from −8 °C. It may then not be easy to estimate this parameter.

- The sensitivity to conductivities at negatives temperatures (−8, −6, −4 and −2 °C) are clearly showing a linear dependency (same pattern) which is likely to make their simultaneous estimation difficult.

From these observations the following conclusions can be drawn:

1. In order to improve the sensitivity to conductivities at positive temperatures and thus their accurate estimation, the heating power and/or heating duration can be increased (to create a higher temperature gradient).
2. Although the highest number of estimated conductivities the better approximation of the actual curve $k = f(\text{temperature})$, it seems that due to sensitivity coefficients correlation, it is only possible to estimate a limited number of points on that curve at a time. This is easily overcome by estimating different sets of conductivities through repeated simulation runs.

5. Conductivity estimation

Simulations using calculated data (probe temperature) to which noise (measurement errors) has been added to simulate real temperatures, have been carried out to study the potential of the method. Measured probe temperatures have been simulated using the values of the sample thermal conductivity shown in Table 1 [20]. In all parameter estimation techniques initial values of the unknown parameters should be chosen carefully for the method to converge. The physical understanding of the direct problem can help setting these values. For example, in this study, initial values have been chosen within the range between the known thermal conductivities of ice and water. These values have also been used as base values for the sensitivity study.

In order to avoid oscillations and divergence of the estimation process, Eq. (13) based on ordinary least squares is modified by a combination of Levenberg method and modified Box–Kanemasu method [17]. The iteration process becomes:

$$\boldsymbol{\beta}^{(k+1)} = \boldsymbol{\beta}^{(k)} + \omega^{(k+1)}\mathbf{P}^{(k)}[\mathbf{X}^{\mathrm{T}(k)}(\mathbf{Y} - \mathbf{T}^{(k)}(\boldsymbol{\beta}))], \tag{14}$$

where ω is a relaxation coefficient calculated by the modified Box–Kanemasu method to avoid oscillations by ensuring that $S\boldsymbol{\beta}^{(k+1)} \leqslant S\boldsymbol{\beta}^{(k)}$ and $\mathbf{P}^{-1} = \mathbf{X}^{\mathrm{T}}\mathbf{X} + \boldsymbol{\Omega}$ with $\boldsymbol{\Omega}$ a diagonal matrix.

From Eq. (14) we note that, near the solution when $\Delta\boldsymbol{\beta} \to 0$ ($\boldsymbol{\beta}^{(k+1)} \approx \boldsymbol{\beta}^{(k)}$), the matrix $\boldsymbol{\Omega}$ has almost no influence on the function S. Therefore this matrix stabilizes the estimation procedure without affecting the solution.

The calculation of $\boldsymbol{\Omega}$ has been proposed in [18]:

$$\Omega_{jj} = \delta \frac{\partial S/\partial \beta_j}{(\partial S/\partial \beta_j)_{\text{init}}} X_{jj}, \tag{15}$$

where δ is a small number, usually $10^{-3} \leqslant \delta \leqslant 10^{-1}$, $\partial S/\partial \beta_j$ is the first derivative of $S(\boldsymbol{\beta})$ with respect to β_j and $(\partial S/\partial \beta_j)_{\text{init}}$ is the first derivative of $S(\boldsymbol{\beta})$ with respect to β_j at the first iteration.

Different numbers of conductivities at different temperatures have been estimated, some of the results are shown in Tables 2–4 (σ being the standard deviation of the added noise, ranging from 0.00 when no noise has been added to 0.15 to include typical experimental errors).

Table 2
Results for three estimated conductivities

Conductivities	$\sigma = 0.00$	$\sigma = 0.02$	$\sigma = 0.08$	$\sigma = 0.15$
k (−5 °C)	2.335	2.338	2.348	2.357
k (−3 °C)	1.790	1.781	1.787	1.723
k (−1 °C)	1.515	1.522	1.532	1.568

Table 3
Results for four estimated conductivities

Conductivities	$\sigma = 0.00$	$\sigma = 0.02$	$\sigma = 0.08$	$\sigma = 0.15$
k (−6 °C)	2.349	2.354	2.365	2.348
k (−3 °C)	1.949	1.939	1.942	1.960
k (−2 °C)	1.576	1.579	1.556	1.477
k (−0.4 °C)	1.130	1.132	1.146	1.379

Table 4
Results for five estimated conductivities

Conductivities	$\sigma = 0.00$	$\sigma = 0.02$	$\sigma = 0.08$	$\sigma = 0.15$
k (−5 °C)	2.301	2.298	2.298	–
k (−4 °C)	2.167	2.219	2.227	–
k (−3 °C)	1.922	1.910	1.910	–
k (−2 °C)	1.582	1.596	1.551	–
k (−0.4 °C)	1.123	1.112	1.164	–

6. Analysis of results

The estimation of fewer parameters does not cause any convergence difficulties (results for 1 and 2 parameters are not shown here). However, estimating fewer points in the curve $k = f(T)$ leads to a loss of accuracy. For example, when $\sigma = 0.00$, estimation error for k (−3 °C) decreases from −5.79% (three parameters) to 1.15% (five parameters). At the same time the accuracy of estimated conductivities is affected by measurement errors (e.g. 2.57% for $\sigma = 0.00$ to 3.15% for $\sigma = 0.15$ on the value of

Table 1
Thermal conductivity of water–agar gel

T (°C)	−10	−5	−4	−3	−2.5	−2	−1.5	−1	−0.4	0
k (W/m K)	2.45	2.30	2.18	1.90	1.76	1.65	1.54	1.40	1.20	0.56

k (-3 °C)). This effect increases with the number of estimated parameters until it becomes impossible for the estimation process to converge (in this case five parameters with maximum noise).

7. Conclusion

The potential of the thermal probe in non-linear conductivity determination has been shown. This has been done through a numerical heat transfer model and an original parameter estimation technique. The mathematical formulation of the system uses enthalpy as primary variable in order to easily accommodate phase change problems. The parameter estimation process minimizes oscillations through controlled relaxation and helps convergence by re-conditioning of the matrix $\mathbf{X}^{\mathrm{T}}\mathbf{X}$. Sensitivity study is crucial in any parameter estimation problem as it provides indications on whether the estimation is possible and the best configuration (e.g. heating power, time, number of parameters etc.). Results so far are very promising and the experimental application of this method will be reported in a following paper.

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