

# A method to determine the thermal conductivity from measured temperature profiles

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(Received 30 September 1988 and in final form 23 November 1988)

**Abstract**—A numerical method to determine the thermal conductivity of a homogeneous material from measured temperature profiles is presented. The problem is formulated as an optimization problem where the heat equation appears as a constraint. This optimization problem is solved with the Davidon–Fletcher–Powell method and in each iteration the heat equation is solved by finite element techniques with the predictor–corrector method.

## 1. INTRODUCTION

DURING the last few decades a lot of efficient numerical methods have been developed for the numerical solution of initial and boundary value problems in physics and applied sciences. The main emphasis in the research on numerical analysis has been on developing accurate methods. In both theoretical and practical applications of numerical methods it is usually assumed that the physical parameters appearing in the models are accurately known. In practice, however, this is rarely the case. Hence, it does not seem to be reasonable to solve the problem with too accurate a numerical method to get satisfactory results. In many cases it also turns out that the exact determination of the model of the physical phenomenon is a much more difficult problem than the actual approximate solution of the model. Often in practical situations measurements are made of temperature, magnetic field, etc. and from these results one would like to estimate a physical quantity so that it fits the measured data. This kind of (mathematically ill-posed) problem has recently received due attention [1–4].

This paper discusses the determination of the thermal conductivity of a homogeneous material from the measured temperatures at certain (finitely many) points. Suppose that other thermal characteristics of the material are known. In most of the studies so far (see the cited papers and their references) the heat conductivity is assumed to be a function of the space coordinate only. This work discusses the situation where the thermal conductivity is dependent on the temperature.

The identification of the thermal conductivity using measured temperature values at well sites is an important inverse problem. A common identification strategy is the indirect one where one minimizes the deviation between a computed solution and the obser-

vations via an iterative process. Alternatively, in steady state the thermal conductivity is sometimes identified by a direct approach [2].

The main difficulty in this kind of problem is that there are usually so few observations that one cannot evaluate the spatial derivative of the temperature by simple numerical differentiation. Hence, heavier and more time-consuming optimization techniques are needed to obtain reliable results.

## 2. THE EXPERIMENTAL SET-UP

In order to estimate the conductivity one can perform for example a heating and cooling experiment. Suppose that we have an experimental apparatus as in Fig. 1, representing the casting of metal. The diameter of the casting is 140 mm and the height is 75 mm. A number of thermocouples are placed at the centreline of the isolated cylinder at varying distances from the

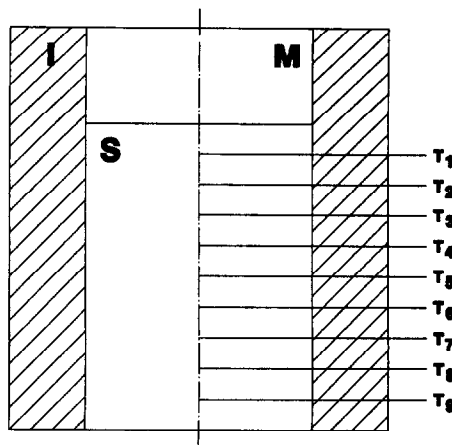


Fig. 1. Schematic sketch of the experimental set-up: I, insulator; M, melted metal; S, mould; and  $T_1, T_2, \dots, T_9$ , thermocouples.

## NOMENCLATURE

$a$	boundary point [m]	$U$	approximation of the temperatures [K]
$b$	boundary point [m]	$U_n$	approximation of the temperatures [K]
$c$	specific heat [ $\text{J kg}^{-1} \text{K}^{-1}$ ]	$v$	test function
$D_j$	approximation of the inverse of the Hessian matrix	$V_h$	test function class
$f$	boundary temperature [K]	$V_h^0$	test function class
$g$	boundary temperature [K]	$W_n$	approximation of the temperature [K]
$h$	grid parameter [m]	$x$	distance [m]
$i$	dummy variable	$x_i$	position of the thermocouple [m]
$I$	objective function [ $\text{K}^2$ ]		
$\tilde{I}$	objective function [ $\text{K}^2$ ]		
$j$	dummy variable		
$k$	dummy variable		
$k_i$	degree of polynomial		
$K$	stiffness matrix		
$M$	mass matrix		
$r$	initial temperature [K]		
$t$	time [s]		
$t_j$	time coordinate of the measuring point [s]		
$\Delta t$	time interval [s]		
$T$	final time [s]		
$u$	temperature [K]		
$\tilde{u}$	measured temperature [K]		
$u(x_i, t_j)$	calculated temperature [K]		

## Greek symbols

$\alpha$	temperature [K]
$\alpha_i$	temperature at different positions [K]
$\beta$	number of temperature intervals
$\eta$	number of the time level
$\kappa$	number of thermocouples
$\lambda$	thermal conductivity [ $\text{J m}^{-1} \text{s}^{-1} \text{K}^{-1}$ ]
$\lambda_{ij}$	approximation of thermal conductivity [ $\text{J m}^{-1} \text{s}^{-1} \text{K}^{-1}$ ]
$\lambda_{\text{opt}}$	calculated thermal conductivity [ $\text{J m}^{-1} \text{s}^{-1} \text{K}^{-1}$ ]
$\lambda_0$	initial thermal conductivity [ $\text{J m}^{-1} \text{s}^{-1} \text{K}^{-1}$ ]
$\rho$	density [ $\text{kg m}^{-3}$ ]
$\varphi_j$	linear basic function.

interface of the melted metal and mould, the thermal conductivity of which is to be determined. After confirming that all thermocouples indicate room temperature, melted metal is poured in. Data of the mould temperature is then stored in the array  $\tilde{u}(x_i, t_j)$ , where  $x_i, i = 1, \dots, \kappa$  is the distance of the  $i$ th thermocouple from the casting and  $t_j, j = 0, \dots, \eta$  is the time after pouring, being expressed by  $t_j = j\Delta t$ , i.e. the temperatures are measured at even time intervals until the final measuring time is reached. The actual distance of each thermocouple from the interface is measured with a depth-micrometer after solidification by carefully scraping away the mould until the thermocouples were exposed.

## 3. THE GOVERNING EQUATION

We assume that the temperature distribution in the mould can be calculated from the one-dimensional heat conduction equation, i.e. the absolute temperature  $u = u(x, t)$  in the material depends only on one space variable  $x$  (the depth) and the time variable  $t$ . Assuming that the boundary values and the initial temperature distribution are given, the governing non-linear partial differential equation can be written in the form

$$\rho c(u) \frac{\partial u}{\partial t} = \frac{\partial}{\partial x} \left( \lambda(u) \frac{\partial u}{\partial x} \right), \quad a < x < b, \quad 0 < t \leq T$$

$$u(a, t) = f(t), \quad 0 \leq t \leq T$$

$$u(b, t) = g(t), \quad 0 \leq t \leq T$$

$$u(x, 0) = r(x), \quad a < x < b. \quad (1)$$

Here the temperature-dependent specific heat  $c(u)$  and the constant density  $\rho$  are assumed to be known, so only the thermal conductivity  $\lambda(u)$  of the material remains to be identified.

## 4. STATEMENT OF THE PROBLEM

Assume that we know the temperatures  $\tilde{u}(x_i, t_j)$  at the points  $x_i, i = 1, \dots, \kappa$  at time levels  $t_j, j = 0, \dots, \eta (= T/\Delta t)$  from the measurements described earlier. Then the problem is to find the thermal conductivity  $\lambda(u)$  such that the solution  $u = u(x, t)$  of equations (1) is a good approximation to the measured values at each time level. Obviously the real thermal conductivity is a solution (though not the only solution) to the following optimization problem: find the function  $\lambda(u)$  which minimizes

$$I(\lambda) = \sum_{i=1}^{\kappa} \sum_{j=0}^{\eta} (\tilde{u}(x_i, t_j) - u(x_i, t_j))^2 \quad (2)$$

where  $u$  satisfies equations (1). Our numerical algorithm will be based on this optimization principle.

## 5. THE NUMERICAL ALGORITHM

To solve the problem we will approximate both the thermal conductivity and the solution  $u(x, t)$  of the

heat equation. This leads to non-linear differential equations which will be solved by predictor–corrector techniques. The thermal conductivity  $\lambda(u)$  is approximated by a piecewise polynomial function

$$\lambda(u) = \lambda_{i0} + \lambda_{i1}u + \dots + \lambda_{ik_i}u^{k_i}, \quad u \in (u_i, u_{i+1}),$$

$$i = 1, \dots, \beta \quad (3)$$

where the temperature interval is divided into  $\beta$  sub-intervals.

The finite element method with linear elements on a uniform grid is used for solving the constraint equations (1) numerically. The finite element basis functions are defined by

$$\varphi_j(x) = \begin{cases} (x - x_{j-1})/h, & x_{j-1} \leq x \leq x_j \\ (x_{j+1} - x)/h, & x_j \leq x \leq x_{j+1} \\ 0, & \text{elsewhere} \end{cases} \quad (4)$$

where  $x_j = a + jh$ ,  $j = 0, \dots, N$  and  $h = (b - a)/N$ . The basis functions span the  $(N + 1)$ -dimensional space  $V_h$ . The solution  $u = u(x, t)$  of equations (1) is approximated by a linear combination of functions  $\varphi_j(x)$

$$u(x, t) \approx U(x, t) = \sum_{j=0}^N \alpha_j(t) \varphi_j(x) \quad (5)$$

with boundary values  $\alpha_0(t) = f(t)$ ,  $\alpha_N(t) = g(t)$ ,  $0 \leq t \leq T$ . Our numerical method can thus be stated as follows: find the thermal conductivity parameters

$$\Lambda = (\lambda_{10}, \dots, \lambda_{1k_1}, \dots, \lambda_{\beta 0}, \dots, \lambda_{\beta k_\beta})$$

that minimize the objective function

$$\tilde{I}(\lambda_{10}, \dots, \lambda_{1k_1}, \dots, \lambda_{\beta 0}, \dots, \lambda_{\beta k_\beta}) = \sum_{i=1}^{\kappa} \sum_{j=0}^{\eta} (\tilde{u}(x_i, t_j) - U(x_i, t_j))^2 \quad (6)$$

where  $U(\cdot, t) \in V_h$  satisfies for each  $t$  the above boundary conditions and the following additional constraints:

$$\rho \int_a^b c(U) \frac{\partial U(x, t)}{\partial t} v(x) dx + \int_a^b \lambda(U) \frac{\partial U(x, t)}{\partial x} \frac{\partial v(x)}{\partial x} dx = 0, \quad \forall v \in V_h^0, t > 0$$

$$\int_a^b U(x, 0) v(x) dx = \int_a^b r(x) v(x) dx, \quad \forall v \in V_h^0, t = 0 \quad (7)$$

where  $V_h^0 = \{v \in V_h : v(a) = v(b) = 0\}$ . In practice, the boundary and initial values are expressed by least-square polynomial fittings of the actual discrete data.

System (7) is actually an initial value problem for a set of non-linear ordinary differential equations of the form

$$M(\alpha, t) \frac{\partial \alpha(t)}{\partial t} + K(\alpha, t) \alpha(t) = 0, \quad t > 0$$

$$M_0 \alpha(0) = U_0, \quad t = 0 \quad (8)$$

where

$$(M(\alpha, t))_{ij} = \rho \int_a^b c(\alpha) \varphi_i(x) \varphi_j(x) dx$$

$$(K(\alpha, t))_{ij} = \int_a^b \lambda(\alpha) \frac{\partial \varphi_i(x)}{\partial x} \frac{\partial \varphi_j(x)}{\partial x} dx$$

$$(M_0)_{ij} = \rho \int_a^b \varphi_i(x) \varphi_j(x) dx$$

$$(U_0)_j = \int_a^b r(x) \varphi_j(x) dx. \quad (9)$$

In the computations, the mass matrix  $M(\alpha, t)$  is evaluated numerically using the Simpson rule, while the stiffness matrix  $K(\alpha, t)$  is computed using the trapezoidal rule.

Equations (8) are finally discretized using the standard Crank–Nicolson method with equal time stepping. Let  $t_n = nk$  and denote  $f(t_n)$  by  $f_n$ . To avoid solving a non-linear algebraic system at every time step the predictor–corrector techniques were used, where the original problem was transformed into two linear systems

$$M(\alpha_n) \frac{\mathbf{W}_{n+1} - \alpha_n}{k} + \frac{1}{2} K_1(\alpha_n) (\mathbf{W}_{n+1} + \alpha_n) = 0,$$

$$n = 0, \dots, T/k - 1$$

$$M\left(\frac{1}{2}(\mathbf{W}_{n+1} + \alpha_n)\right) \frac{\alpha_{n+1} - \alpha_n}{k} + \frac{1}{2} K_1\left(\frac{1}{2}(\mathbf{W}_{n+1} + \alpha_n)\right) (\alpha_{n+1} + \alpha_n) = 0$$

$$n = 0, \dots, T/k - 1$$

$$M_0 \alpha_0 = U_0. \quad (10)$$

A more detailed study of the algorithm can be found in ref. [5].

## 6. OPTIMIZATION METHOD

To solve the optimization problem the Davidon–Fletcher–Powell method (cf. ref. [4]) was used. The basic idea is that the search directions are of the form  $-D_j \nabla I(\lambda)$ . The numerically calculated gradient direction is thus deflected by premultiplying it by  $D_j$ , where  $D_j$  is an  $n \times n$  positive definite symmetric matrix that approximates the inverse of the Hessian matrix. For the purpose of the next step,  $D_{j+1}$  is formed by adding two symmetric matrices, each of rank one, to  $D_j$ . In particular, if the objective function is quadratic, then the method yields conjugate directions [4]. The gradient direction is calculated numerically by computing the change of the objective function corresponding to a small change in each  $\lambda_{ij}$ . Obviously this is the most time-consuming step in the algorithm.

## 7. TEST PROBLEMS

We analyse here some test problems with the above algorithm. The exact solution of Example 1 is taken as  $\tilde{u}(x_i, t_j)$ .

*Example 1*

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x} \left( \frac{\partial u}{\partial x} \right), \quad 0 < x < 1, 0 < t \leq 0.1$$

$$u(0, t) = 0, \quad 0 \leq t \leq 0.1$$

$$u(1, t) = 0, \quad 0 \leq t \leq 0.1$$

$$u(x, 0) = \sin(\pi x), \quad 0 < x < 1$$

at  $x_i = i/7, i = 0, \dots, 7, t_j = 0.01j, j = 0, \dots, 10$ . The exact temperature is in this case

$$u(x, t) = e^{-\pi^2 t} \sin(\pi x).$$

To solve the constraint equation the time step  $k = 0.01$  is chosen and the interval  $0 \leq x \leq 1$  is divided into 20 subintervals, i.e.  $N = 20$ . We approximate first the thermal conductivity by a polynomial of degree two in the whole temperature interval  $0 \leq u \leq 1$ . The initial guess is taken as

$$\lambda_0(u) = 5 + 5u + 5u^2, \quad 0 \leq u \leq 1.$$

After optimization, the value of the objective function reaches a minimum at

$$\lambda_{\text{opt}}(u) = 0.991 + 0.010u - 0.037u^2, \quad 0 \leq u \leq 1$$

and the value of the objective function is  $\tilde{I}(\lambda_{\text{opt}}) = 0.830 \times 10^{-4}$ .

The algorithm does not, however, work for all initial guesses. For example if we choose the initial approximation  $\lambda_0(u) = 5$ , the algorithm works if  $\lambda(u)$  is restricted to a constant, but no reasonable solution is found from among the quadratic polynomials. Hence we see that one should keep a careful balance between the inaccuracy of the initial guess and the number of free parameters used.

Next, let us approximate the thermal conductivity with a piecewise constant function. The temperature interval is divided into three subintervals and the initial guess is chosen as

$$\lambda_0 = 5.000, \quad \text{when } 0.000 \leq u < 0.333$$

$$\lambda_0 = 5.000, \quad \text{when } 0.333 \leq u < 0.667$$

$$\lambda_0 = 5.000, \quad \text{when } 0.667 \leq u \leq 1.000.$$

In this case the algorithm is terminated when the thermal conductivity is

$$\lambda_{\text{opt}} = 0.991, \quad \text{when } 0.000 \leq u < 0.333$$

$$\lambda_{\text{opt}} = 0.989, \quad \text{when } 0.333 \leq u < 0.667$$

$$\lambda_{\text{opt}} = 0.973, \quad \text{when } 0.667 \leq u \leq 1.000$$

and the value of the objective function is  $\tilde{I}(\lambda_{\text{opt}}) = 0.815 \times 10^{-4}$ . Also the initial guesses  $\lambda_0(u) = 3$  and 0 lead to the same value, but when we

have the guess  $\lambda_0(u) = 5$  and the temperature intervals are for example (0, 0.323), (0.323, 0.489), (0.489, 1), the algorithm again does not give a reasonable solution. We finally note that the piecewise constant approximation is quite sensitive to the choice of temperature intervals.

In the second example (Example 2) the thermal conductivity is not constant.

*Example 2*

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x} \left( (1+u) \frac{\partial u}{\partial x} \right) - \pi^2 \cos(2\pi x) e^{-2\pi^2 t},$$

$$0 < x < 1, 0 < t \leq 0.1$$

$$u(0, t) = 0, \quad 0 \leq t \leq 0.1$$

$$u(1, t) = 0, \quad 0 \leq t \leq 0.1$$

$$u(x, 0) = \sin(\pi x), \quad 0 < x < 1.$$

The exact solution, the observation points, the number of subintervals and the time step are the same as in the previous example. We approximate first the thermal conductivity with a second-degree polynomial in the whole temperature interval. The initial guess is the same as in Example 1. The minimum value of the objective function is in this case  $\tilde{I}(\lambda_{\text{opt}}) = 0.654 \times 10^{-4}$  for the thermal conductivity

$$\lambda_{\text{opt}}(u) = 0.993 + 1.000u - 0.003u^2, \quad 0 \leq u \leq 1.$$

Also the initial guesses  $\lambda_0(u) = 10$  and 0 lead to the same solution, but with the guess  $\lambda_0(u) = 5$  the algorithm cannot find a reasonable solution even if the quadratic term is omitted.

Assuming the initial guess  $\lambda_0(u) = 5$  in a piecewise constant approximation, the algorithm converges to  $\tilde{I}(\lambda_{\text{opt}}) = 0.734 \times 10^{-3}$  where

$$\lambda_{\text{opt}} = 1.129, \quad \text{when } 0.000 \leq u < 0.333$$

$$\lambda_{\text{opt}} = 1.490, \quad \text{when } 0.333 \leq u < 0.667$$

$$\lambda_{\text{opt}} = 1.748, \quad \text{when } 0.667 \leq u \leq 1.000.$$

The initial guesses  $\lambda_0(u) = 3$  and 1 lead to the same solution, but with the guess  $\lambda_0(u) = 0$  the algorithm fails. When the temperature intervals are (0, 0.323), (0.323, 0.489), (0.489, 1) the algorithm finds a reasonable solution also with the initial guess  $\lambda_0(u) = 0$ .

If we choose polynomials other than constant in the piecewise approximation, the algorithm does not work properly. In that case the algorithm becomes very sensitive to the choice of initial values and to the number of observation points in each temperature interval. So it is better to seek the thermal conductivity in the whole temperature interval, if there are only a few points where the temperature is measured. It is also important that the heat conduction process is not near the steady-state situation, where every constant thermal conductivity is a solution to the optimization problem.

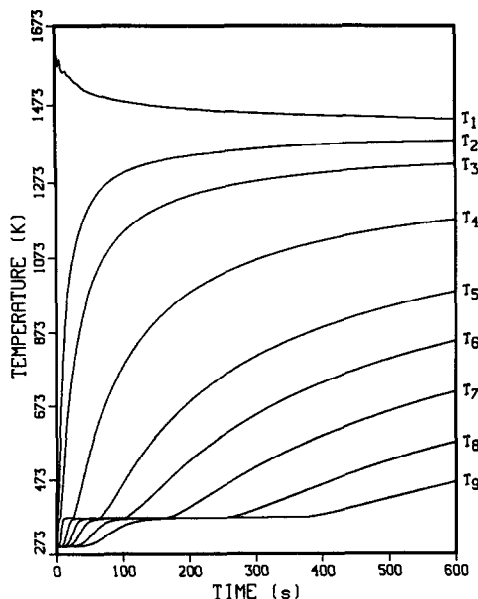


FIG. 2. The temperatures of the thermocouples  $T_i$ ,  $i = 1, \dots, 9$ .

## 8. A PRACTICAL EXAMPLE

Our practical problem is to determine the thermal conductivity of the mould sand in Fig. 1. The sand which was investigated consists of 85.2% quartz, 3.3% coal, 8.0% bentonite and 3.5% water. Only temperatures above 373 K are considered so we can assume that there is no moisture left. Moreover, the effect of the phase transition from  $\alpha$ -quartz to  $\beta$ -quartz at 848 K is neglected since the energy involved is small [4]. Indeed, no constant-temperature phase transition zone can be seen from the heating curves in Fig. 2. The specific heat of the sand is calculated by a weighted average of its components, and for the components we use the values given in ref. [7]. The density of the sand is assumed to be  $\rho = 1530 \text{ kg m}^{-3}$  independent of the temperature. Nine thermocouples  $T_i$ ,  $i = 1, \dots, 9$  were used in the experimental apparatus and the temperatures were observed every 1.25 s. The initial condition of the constraint equation is a least-square fit to the temperatures measured 185 s after the beginning of the cast. The boundary conditions are also least-square approximations of the temperatures of the thermocouples  $T_1$  and  $T_7$ . Thus seven thermocouples were in the area where temperature are over 373 K. They were placed 0, 2.9, 3.8, 8.0, 13.1, 16.6 and 20.6 mm from the metal-mould interface. Ideally, we would like to start the simulation at the same time as casting begins. The problem is then that most thermocouples in the sand have temperatures below 373 K. The most interesting phenomena appear before the time level 600 s, because after this the temperature distribution is near the steady state. The investigation was extended to three different final times, namely  $T = 200, 300$  and 400 s, to compare the results. The interval between the position of thermocouples  $T_1$  and

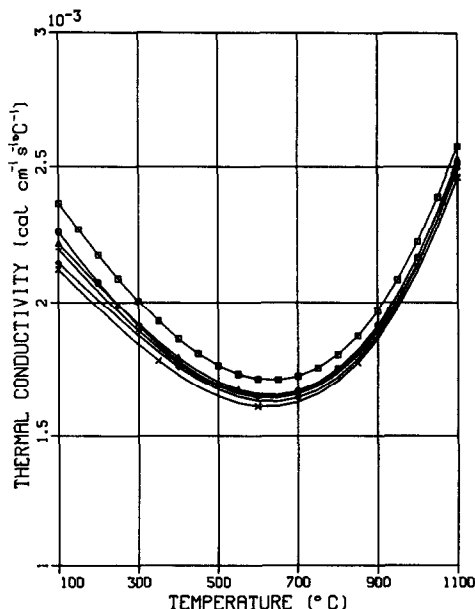


FIG. 3. The thermal conductivity of the investigated sand. The final times of the calculation are with initial guess  $\lambda_0(u) = 1.0$ :  $\circ$ , 200;  $\triangle$ , 300;  $\diamond$ , 400 s and with initial guess  $\lambda_0(u) = 0.4$ :  $\square$ , 200;  $\times$ , 300;  $\nabla$ , 400 s.

$T_7$  was divided into  $N = 20$  subintervals and the time step in the numerical scheme was chosen to be  $k = 1.25$  s. The thermal conductivity was approximated by a cubic polynomial function in the whole temperature interval. The initial guesses were  $\lambda_0(u) = 1$  and 0.4 in each case. The results of the algorithm are presented in Fig. 3. We note that the curves do not differ much from each other. The r.m.s. difference between the calculated and measured temperatures varies from 10.96 to 11.83 K. The thermal conductivity curves in Fig. 3 have the same shape and magnitude as those in refs. [3, 4].

## 9. DISCUSSION

The problem considered in this paper is mathematically ill-posed and its solution by the above method has a disadvantage that it needs quite a lot of computer time and the solution depends on the position of the thermocouples. To minimize computing time there are at least three possibilities: approximating the thermal conductivity with fewer parameters, improving optimization techniques and providing a good initial guess. In the practical calculation the piecewise constant approximation was not as useful as polynomials in the whole temperature interval. The results depend heavily on the length of the temperature intervals, i.e. the number of measuring points in each interval. Also in the situation where the initial temperature distribution is a rough function of the space variable and there are only few observation points, the algorithm does not work properly. The problem of a non-unique solution can occur near the steady-state situation. Moreover, the

objective function is not always convex and so there are local minima to make the problem more difficult and expensive to solve. One should also note that the spatial differencing in the numerical solution of the heat equation should in general be fine enough (as compared with the intervals between the thermocouples) to get meaningful results. The sensitivity of the algorithm with respect to the initial guess can be reduced by starting from low-order approximations which are relatively stable numerically.

If we want the solution to be smooth it might be useful to insert some penalty terms to the objective function which would depend on, for example, the derivative of the solution with respect to the space variable. These kind of techniques have been investigated in ref. [8]. In the case of the practical example discussed above, this work does not give an answer to the question how the moisture of the sand influences the investigated physical property, because in that situation the kind of model discussed here does not hold any more. New constraint equations are needed at temperatures near 373 K to model the phase change of water.

*Acknowledgment*—The author would like to thank Prof. J. Pitkäranta and Dr R. Stenberg for several helpful suggestions which contributed substantially to the development of this paper.

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## METHODE DE DETERMINATION DE LA CONDUCTIVITE THERMIQUE A PARTIR DE PROFILS MESURES DE TEMPERATURE

**Résumé**—On présente une méthode numérique pour déterminer la conductivité thermique d'un matériau homogène à partir de profils mesurés de température. Ceci est présenté comme un problème d'optimisation dans lequel l'équation de la chaleur apparaît comme une contrainte. Ce problème d'optimisation est résolu par la méthode Davidon–Fletcher–Powell et dans chaque itération l'équation de la chaleur est résolue par une technique d'éléments finis avec une méthode de prédiction–correction.

## METHODE ZUR BESTIMMUNG DER WÄRMELEITFÄHIGKEIT AUS GEMESSENEN TEMPERATURPROFILEN

**Zusammenfassung**—Ein numerisches Verfahren zur Bestimmung der Wärmeleitfähigkeit eines homogenen Materials aus gemessenen Temperaturprofilen wird vorgestellt. Bei dem entstehenden Optimierungsproblem erscheint die Wärmeleitgleichung als Randbedingung. Zur Optimierung wird die Davidon–Fletcher–Powell-Methode verwendet, wobei in jedem Iterationsschritt die Wärmeleitgleichung durch die Kombination von Finite-Elemente-Methoden und einer Technik mit Schätzung und verbesserter Schätzung gelöst wird.

## МЕТОД ОПРЕДЕЛЕНИЯ ТЕПЛОПРОВОДНОСТИ ПО ИЗМЕРЕННЫМ ПРОФИЛЯМ ТЕМПЕРАТУРЫ

**Аннотация**—Предложен численный метод определения теплопроводности однородного материала по измеренным профилям температуры. Проблема формулируется как задача оптимизации, в которой в качестве ограничения используется уравнение теплопроводности. Задача решается методом Дэвидона–Флетчера–Пауэлла. На каждой итерации уравнение теплопроводности решается методом конечных элементов с использованием предиктор–корректора.