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IDENTIFICATION OF BASIC THERMAL TECHNICAL CHARACTERISTICS OF BUILDING MATERIALS

STANISLAV ŠŤASTNÍK, JIŘÍ VALA AND HANA KMÍNOVÁ

Modelling of building heat transfer needs two basic material characteristics: heat conduction factor and thermal capacity. Under some simplifications these two factors can be determined from a rather simple equipment, generating heat from one of two aluminium plates into the material sample and recording temperature on the contacts between the sample and the plates. However, the numerical evaluation of both characteristics leads to a non-trivial optimization problem. This article suggests an efficient numerical algorithm for its solution, based on the weak formulation of certain initial and boundary problem for the heat transfer equation, on the classical Fourier analysis and on the Newton iterative method, and demonstrates its practical application.

Keywords: building heat transfer, PDEs of evolution, inverse problems, Fourier method, Newton iterations, uncertainties in laboratory measurements

AMS Subject Classification: 80A20, 80A23, 42A16, 65T40, 65K10

1. INTRODUCTION

Mathematical and numerical modelling of heat transfer (conduction, convection and radiation) in buildings, based on conservation laws of classical mechanics, needs at least the following characteristics of all applied materials: their densities ρ [kg/m^3], their heat conduction factor λ [$\text{W}/(\text{K m})$] and (if some non-stationary processes are taken into account) their thermal capacity c [$\text{J}/(\text{K kg})$]. The density of a dry material sample can be determined easily from its volume and mass (mediated by its weight). The identification of a remaining couple of characteristics, introduced properly e. g. in [12], pp. 52, 57, is more delicate because most building materials have complicated porous structures and both practical observation and laboratory measurements suffer from the their absorptivity, namely in such equipments where the presence of water or air humidity (in various phases) cannot be excluded: λ for water is 20-times greater than that λ for dry air (cf. [18], p. 36). This is also the case of setting λ from the measurement of stationary heat transfer and c from some common calorimeter system. Therefore a new (rather simple) equipment was suggested at the Department of Technology of Building Materials and Components of the Faculty of Civil Engineering of the Brno University of Technology; its more detailed description has been published in [11]. It consists of two thin aluminium plates, encased by insulation blocks, made from the polystyrene foam. In the zero

time the temperature is constant everywhere, then one of the plates (the right-hand one here) begins to act as a heating unit. The material sample (whose characteristics λ and c are not known in advance) is fixed between the plates. The values of temperature T [K] in time t [s] are obtained from two sensors located on the contacts between the sample and the plates. Our final aim is to reconstruct (as accurately as possible) the values of λ and c from this information.

It is clear that the validity of results, received by above sketched measurements, is limited. The advanced design of modern buildings should involve so-called HAM (“heat, air and moisture”) analysis where the (relatively quick) heat propagation is conditioned by very slow redistribution of moisture (and facultative contaminants) both in construction parts of a building and in air in rooms; the corresponding mathematical models, based on physical laws of conservation of mass, momentum (3 components) and energy (for more details see [7], p. 4, and [18], p. 38), and numerical algorithms should involve such processes as Navier–Stokes compressible air flow, moisture redistribution due to irreversible sorption isotherms, etc. Moreover, some “effective” material properties should be explained as limit values by an appropriate homogenization (e. g. two-scale convergence) technique. The classical Fourier continuity equation (cf. [4], p. 263), assumes that all materials are (at least macroscopically, in sense of “effective” values) homogeneous, isotropic, dry (without any moisture or contaminants) and that their characteristics $\zeta = \rho c$ and λ are independent of T . In real buildings this is often not true; nevertheless, it is important to have some reliable values of λ and c , (like “representative values” from [4], p. 28, for a lot of materials, frequently used in civil engineering), at least for first rough calculations, forced by thermal technical standards, namely in case of material design and laboratory testing of new insulation layers.

2. HEAT TRANSFER EQUATION

In addition to above mentioned simplifications, let us consider the heat transfer only in one direction x [m]. Let us suppose that the generated heat r [W/m³] by a heating unit is a bounded real-valued function of t , constant in x , and that no heat flow are present on outer surfaces of insulation blocks (in practice, long-time experiments are not allowed). For certain real lengths l , L and H the following materials for $-H \leq x \leq H$ will be considered:

- the tested material for $|x| \leq l$,
- the aluminium plates for $l < |x| < L$, $\delta = L - l$, $\bar{l} = \frac{1}{2}(l + L)$,
- the polystyrene blocks for $L \leq |x| \leq H$, $h = H - L$, $\bar{L} = \frac{1}{2}(L + H)$

(the position of sharp inequalities here is only formal, quite unsubstantial). Instead of c we shall make use of ζ only (if necessary, we can calculate $c = \zeta/\rho$ a posteriori). To distinguish between the corresponding values of material characteristics in the tested material and in the remaining layers, let us introduce such notation $\tilde{\lambda}$ and $\tilde{\zeta}$ and formally also \tilde{r} that

$$\tilde{\lambda} = \lambda\chi_3 + \lambda_\delta(\chi_2 + \chi_4) + \lambda_h(\chi_1 + \chi_5),$$

$$\begin{aligned} \tilde{\zeta} &= \zeta\chi_3 + \zeta_\delta(\chi_2 + \chi_4) + \zeta_h(\chi_1 + \chi_5), \\ \tilde{r}(t) &= r(t)\chi_4 \end{aligned}$$

where χ_j with $j \in \{1, 2, 3, 4, 5\}$ are characteristic functions of the sets defined by the following relations:

$$\begin{aligned} -H \leq x \leq -L & \text{ for } j = 1, \\ -L < x < -l & \text{ for } j = 2, \\ -l \leq x \leq l & \text{ for } j = 3, \\ l < x < L & \text{ for } j = 4, \\ L \leq x \leq H & \text{ for } j = 5; \end{aligned}$$

$\lambda, \zeta, \lambda_\delta, \zeta_\delta, \lambda_h, \zeta_h$ are considered as positive constants.

Let us assume that T is constant everywhere in the initial time $t = 0$, i. e. for some T_0 we can set simply $T(x, 0) = T_0$ for every admissible x ; Since we are studying a layered material, the differential (strong) formulation of our heat equation is less convenient than the integral (weak) one:

$$(\varphi, \tilde{\zeta}\dot{T}) + (\varphi', \tilde{\lambda}T') = (\varphi, \tilde{r}) \tag{1}$$

for all φ from the Sobolev space $\mathcal{W}^{1,2}(-H, H)$; T has to be found in $\mathcal{W}^{1,2}(-H, H)$, too. The prime symbols represent derivatives by x , the dot symbols derivatives by t , the symbols (\cdot, \cdot) in (1) refer to scalar products in the Lebesgue space $\mathcal{L}^2(-H, H)$. Let us notice that the formal integration of (1) by parts in the variable x (despite the fact that some derivatives are allowed to be considered only in sense of distributions) causes that all boundary integrals at $x = -L, x = -l, x = l$ and $x = L$ give zero sums and that both boundary integrals at $x = -H$ and $x = H$ are equal to zero thanks to the assumption of no heat flows between our system and external environment. Consequently, all needed boundary conditions are hidden in (1).

The existence of a unique T for given $\tilde{\zeta}, \tilde{\lambda}$ and \tilde{r} can be verified easily in various ways, e. g. applying the arguments of the Lax–Milgram theorem for certain time-discretized version of (1) and of the convergence of Rothe sequences, as usual in the numerical analysis of initial and boundary problems of partial differential equations of evolution of parabolic type (cf. [15], p. 157), or, alternatively, exploiting the theory of Fourier integral transform (cf. [1], p. 184). However, our problem is more difficult than to solve (1) directly: we know constant \tilde{r} and also $\tilde{\lambda}$ and $\tilde{\zeta}$ for $|x| > l$ and we have to find λ and ζ for $|x| \leq l$, identical with λ and ζ , from S couples of data T_{s-}, T_{s+} , obtained by two temperature sensors in s different times $t_s, s \in \{1, \dots, S\}$ (theoretically with $S \rightarrow \infty$, in practical calculations with some finite S). We should obtain an optimization problem with explicit unknowns ζ and λ (evidently strongly non-linear, but only in two variables).

3. FOURIER ANALYSIS

Instead of (1) let us consider the same equation restricted to certain x between a_- and a_+ where $-H \leq a_- < a_+ \leq H$ such that $\tilde{\lambda}, \tilde{\zeta}$ and \tilde{r} are constant for all such x 's. Then (1) degenerates to

$$\tilde{\zeta}\langle \tilde{\varphi}, \dot{T} \rangle + \tilde{\lambda}\langle \tilde{\varphi}', T' \rangle = \varphi(a_+)q_+ - \tilde{\varphi}(a_-)q_- + \tilde{r}\langle \tilde{\varphi}, 1 \rangle \tag{2}$$

for all $\tilde{\varphi}$ from $W^{1,2}(a_-, a_+)$; all symbols $\langle \cdot, \cdot \rangle$ here refer to scalar products in $L^2(a_-, a_+)$ and some boundary (time-dependent) thermal fluxes q_- and q_+ , non-zero in general (missing in (1) thanks to our physical assumptions), occur. Following the well-known Fourier method of multiplicative decomposition, let us now replace $T(x, t)$ by

$$T_N(x, t) = T_N(x, t_*) + \sum_{n=0}^N \varphi_n(\tilde{x})\alpha_n(t - t_*), \tag{3}$$

expecting $T_N(x, t_*)$ for some $0 \leq t_* < t$ is a priori known, $T_N(x, t) \rightarrow T(x, t)$ for an integer index $N \rightarrow \infty$; functions $\tilde{\varphi}_n$ of x here form a basis of the finite-dimensional subspace of $W^{1,2}(0, 1)$ and α_n are time-variable functions, satisfying initial conditions $\alpha_n(0) = 0$. Let us introduce $a = a_+ - a_-$; we shall project the elements of $W^{1,2}(a_-, a_+)$ onto $W^{1,2}(0, 1)$. The choice of a function $\varphi_m(\tilde{x})$, $\tilde{x} = (x - a_-)/a$ with $m \in \{0, \dots, N\}$ as $\tilde{\varphi}$ in (2) results

$$\begin{aligned} & \sum_{n=0}^N \left(a\tilde{\zeta}[\varphi_m, \varphi_n]\dot{\alpha}_n + a^{-1}\tilde{\lambda}[\varphi'_m, \varphi'_n]\alpha_n \right) \\ &= \sum_{n=0}^N (\varphi_m(1)q_+ - \varphi_m(0)q_- + a\tilde{r}[\varphi_m, 1]) . \end{aligned} \tag{4}$$

The scalar products $\langle \cdot, \cdot \rangle$ from $L^2(a_-, a_+)$ we have replaced by the analogous ones $[\cdot, \cdot]$ from $L^2(0, 1)$; the prime symbols here represents derivatives by \tilde{x} .

Let us identify the interval (a_-, a_+) , projected onto $(0, 1)$, step by step with our five intervals $(-H, -L)$, $(-L, -l)$, $(-l, l)$, (l, L) and (L, H) . For simplicity let us assume that such regular square matrix M of order $N + 1$, such square matrix K of order $N + 1$ and of rank N and such column vector g of length $N + 1$ exist that $[\varphi_m, \varphi_n]$ (with $m, n \in \{0, \dots, N\}$) generates a matrix M , $[\varphi'_m, \varphi'_n]$ a matrix K and $[\varphi_m, 1]$ a vector g ; both (symmetric) matrices M and K , in general not diagonal, and a vector g consist of some real factors, in general depending on m and n , not on a , and are able to be extended with increasing N easily. Then (4) can be rewritten in the simple matrix form

$$a\tilde{\zeta}M\dot{\alpha} + a^{-1}\tilde{\lambda}K\alpha = \beta_+q_+ - \beta_-q_- + a\tilde{r}g \tag{5}$$

where two column vectors β_-, β_+ of length $N + 1$ consist of values $\varphi_0(0), \dots, \varphi_N(0)$ and $\varphi_0(1), \dots, \varphi_N(1)$ and an unknown column vector α of length $N + 1$ depends on $t - t_*$.

Since (5) is a system of $N + 1$ ordinary differential equations with $N + 1$ unknowns, stored in a vector α , the spectral analysis of could be useful. Let us consider the diagonal matrix Ω , consisting of all eigenvalues ω_n , $n \in \{0, \dots, N\}$, $0 = \omega_0 < \omega_1 < \omega_n$ of the matrix $(\tilde{\lambda}/\tilde{\zeta})M^{-1}K$ (the first equality here follows from the assumption $\text{rank } K = N - 1$, which together with remaining strict inequalities induces certain limitation for the choice of the basis φ_n , $n \in \{0, \dots, N\}$, i. e.

$$\det(\tilde{\lambda}K - a^2\omega_n\tilde{\zeta}M) = 0;$$

thus $\tilde{\lambda}KV = a^2\tilde{\zeta}MV\Omega$ for the matrix V of all column eigenvectors, corresponding to ω_n . It is easy to verify (as e. g. in [17], p.38) that both Ω and V are real matrices and that the matrix V is orthogonal (i. e. $V^{-1} = V^T$).

In practical calculations we cannot rely on our complete knowledge of the right-hand side of (5): q_-, q_+ and \tilde{r} are variable in time, q_-, q_+ are not ready yet (and will have to be determined from four additional continuity conditions for T_N), \tilde{r} is known only in $S + 1$ discrete times (including the initial one) $t_s, s \in \{0, \dots, S\}, 0 = t_0 < t_1 < \dots < t_S$, identical with the adjusting times of the heat source; for $s > 1$ the notation $\tau_s = t_s - t_{s-1}$ will be used frequently. Let us suppose that the temperature measurements are realized for in the same discrete times t_s ; the recorded values will be denoted by T_{s-} for $x = -l$ (the inner surface of the unheated aluminium plate) and T_{s+} for $x = l$ (the inner surface of the heated one). The success of all measurements is conditioned by such their arrangement that all τ_s are sufficiently small: theoretically their maximum tends to zero as $S \rightarrow \infty$. Thus it is natural to consider \tilde{r} (equal to r or zero) and similarly also q_- and q_+ as fixed for $t_{s-1} < t \leq t_s$; the corresponding values will be denoted by \tilde{r}_s, r_s, q_{s-} and q_{s+} . Thus it is natural to start with the analysis of the equation

$$a\tilde{\zeta}M\dot{\alpha} + a^{-1}\tilde{\lambda}K\alpha = a\eta, \tag{6}$$

identical with (5) with the right-hand side replaced by certain constant vector η of length $N + 1$.

We can solve (6) as a system of $N + 1$ ordinary linear differential equations with $N + 1$ unknowns. Using the standard method of variation of constants (analyzed in details e. g. in the textbook [9], p.86) we receive its general solution in the form

$$\alpha(\tau) = V \begin{bmatrix} 1 \\ \exp(-a^2\tilde{\zeta}\omega_1\tau/\tilde{\lambda}) \\ \dots \\ \exp(-a^2\tilde{\zeta}\omega_N\tau/\tilde{\lambda}) \end{bmatrix} \kappa + V \begin{bmatrix} \tau \\ \tilde{\lambda}/(a\tilde{\zeta}\omega_1) \\ \dots \\ \tilde{\lambda}/(a\tilde{\zeta}\omega_N) \end{bmatrix} V^T M^{-1}\eta/(a\tilde{\zeta}).$$

where $\tau = t - t_*$ and κ is a vector of unknown real constants. The application of the initial condition $\alpha(0) = 0$ yields

$$\kappa = - \begin{bmatrix} 0 \\ \tilde{\lambda}/(a^2\tilde{\zeta}\omega_1) \\ \dots \\ \tilde{\lambda}/(a^2\tilde{\zeta}\omega_N) \end{bmatrix} V^T M^{-1}\eta/(a\tilde{\zeta});$$

thus

$$\alpha(\tau) = V \begin{bmatrix} \tau/(a\tilde{\zeta}) & & & \\ & \tilde{\lambda}/(a^2\tilde{\zeta}^2\omega_1)(1 - \exp(-a^2\tilde{\zeta}\omega_1\tau/\tilde{\lambda})) & & \\ & & \ddots & \\ & & & \tilde{\lambda}/(a^2\tilde{\zeta}^2\omega_N)(1 - \exp(-a^2\tilde{\zeta}\omega_N\tau/\tilde{\lambda})) \end{bmatrix} V^T M^{-1} \eta.$$

Consequently we have

$$\alpha(\tau_s) = V\Psi_s(\tilde{\lambda}, \tilde{\zeta})V^T M^{-1} (\beta_{+q_{s+}} - \beta_{-q_{s-}} + \tilde{r}_s g) \tag{7}$$

where the matrix $\Psi_s(\tilde{\lambda}, \tilde{\zeta})$ consists only of diagonal terms

$$\Psi_{0s} = \frac{\tau_s}{a\tilde{\zeta}}, \quad \Psi_{ns} = \frac{\tilde{\lambda}}{a^2\tilde{\zeta}^2\omega_n} \left(1 - \exp\left(-\frac{a^2\tilde{\zeta}\omega_n\tau_s}{\tilde{\lambda}}\right) \right)$$

for $n \in \{1, \dots, N\}$; let us notice that Ψ_{0s} does not depend on $\tilde{\lambda}$ at all and that the first rough approximation (using the MacLaurin polynomial of order 1 instead of the exponential function) is $\Psi_{ns} \approx \Psi_{0s}$. It is also interesting to observe that exactly two positions of $\tilde{\lambda}$ and $\tilde{\zeta}$ can be distinguished here: i) as the ratio $\tilde{\zeta}/\tilde{\lambda}$, identical with the “thermal diffusivity” from [12], p.191, ii) as $\tilde{\zeta}$ separately. If q_{s-} and q_{s+} are given then $T_N(x, t_s)$ can be now calculated easily for any $s \in \{1, \dots, S\}$ from (3), applying $t = t_s$ and $t_* = t_{s-1}$, in the form

$$T_N(x, t_s) = T_N(x, t_{s-1}) + \sum_{n=0}^N \varphi_n(\tilde{x})\alpha_n(\tau_s), \tag{8}$$

where briefly $T_s(x) = T_N(x, t_s)$ (and $T_{s-1}(x) = T_N(x, t_{s-1})$, too), unlike measured T_{s-} or T_{s+} , referring only to $x = -l$ or $x = l$ (evidently for $s = 0$ all these temperatures are equal to T_0).

An alternative approach to the direct solution of (6) seems to be the application of the classical method of discretization in time, based on the Euler implicit formula, i. e. on the modification of (6)

$$a\tilde{\zeta}M(\alpha - \alpha(0)) + a^{-1}\tilde{\lambda}K\alpha = a\eta.$$

However, the solution of this system of $N + 1$ linear algebraic equations

$$\alpha(\tau) = \left(\frac{a\tilde{\zeta}}{\tau} M + \frac{\tilde{\lambda}}{a} K \right)^{-1} \left(\eta + \frac{a\tilde{\zeta}}{\tau} M\alpha(0) \right)$$

for any positive τ contains $\tilde{\lambda}$ and $\tilde{\zeta}$ at unpleasant positions, unsuitable for fast algebraic manipulations. The same drawback occurs also in other numerical methods of common use, based on the discretization in time (whose overview can be found e. g. in [14], p. 219). This prefers the spectral analysis to the algebraic construction of the sequences of Rothe in our application.

must be done only once in practice (for a fixed N the value ϵ is not important), using some efficient numerical algorithm, based on the spectral properties of such matrices, studied in [8], p. 160, e. g. the fast QR -transformation, described in [14], p. 558, yet.

Clearly more complicated (than piecewise linear) basis can be selected; moreover, a lot of other numerical methods is available – our assumptions on certain “special mode” of M and K are not too strong. Even some advanced meshless techniques, including those based on the Fourier, Laplace and other integral transforms (different from the above criticised classical approach), are available; for more information and references see [1], p. 184, and [6], p. 23. Nevertheless, we shall not discuss them in details; our main aim is now to evaluate the temperature, to compare the results for $x \in \{-l, l\}$ with T_{s-} or T_{s+} and to receive some optimization problem for two unknowns λ and ζ . Let us remark that for the derivation of the rather complicated following formulae we have made use of our original software code for symbolic manipulations, supported by several functions of the MATLAB toolbox “symbolic” (referring to the core of MAPLE).

4. INTERFACE HEAT FLUXES

The formulae (7) and (8) for any fixed $s \in \{1, \dots, S\}$ assumes that both interface heat fluxes q_{s-} and q_{s+} are prescribed a priori. However, we know that this is not a realistic situation. On five intervals (identified by $j \in \{1, \dots, 5\}$) we should set ten such unknown parameters; only two of them (for $x = -H$ and $x = H$) are equal to zero by the assumption of missing thermal fluxes between our system and external environment. To overcome this difficulty, we must therefore add eight additional continuity requirements: four on such interface heat fluxes, four on the temperature. These requirements can be formulated in the simple way:

$$\begin{aligned} q_{s-} &= 0, & q_{s+} &= P_{s-}, & a_- &= -H, & a_+ &= -L & \text{for } j &= 1, \\ q_{s-} &= P_{s-}, & q_{s+} &= p_{s-}, & a_- &= -L, & a_+ &= -l & \text{for } j &= 2, \\ q_{s-} &= p_{s-}, & q_{s+} &= p_{s+}, & a_- &= -l, & a_+ &= l & \text{for } j &= 3, \\ q_{s-} &= p_{s+}, & q_{s+} &= P_{s+}, & a_- &= l, & a_+ &= L & \text{for } j &= 4, \\ q_{s-} &= P_{s+}, & q_{s+} &= 0, & a_- &= L, & a_+ &= H & \text{for } j &= 5; \end{aligned}$$

here P_{s-}, p_{s-}, p_{s+} and P_{s+} are (still unknown) real parameters and $T_s(x)$ is forced to be continuous in all points $x \in \{-L, -l, l, L\}$.

We need to determine P_-, p_-, p_+ and P_+ , proportional to r_s , as certain functions $\vartheta_-, \Theta_-, \vartheta_+$ and Θ_+ of λ and ζ , i. e.

$$P_{s-} = \Theta_{s-}ar_s, \quad p_{s-} = \vartheta_{s-}ar_s, \quad p_{s+} = \vartheta_{s+}ar_s, \quad P_{s+} = \Theta_{s+}ar_s.$$

Let us introduce the notation $b = V^T M^{-1}g$, $\psi_- = V^T \beta_-$, $\psi_+ = V^T \beta_+$, $\gamma_- = V^T \beta_-$ and $\gamma_+ = V^T \beta_+$. Then (7) and (8) yield

$$T(a_-, t_s) - T(a_-, t_{s-1}) = \sum_{n=0}^N \Psi_{ns}(\tilde{\lambda}, \tilde{\zeta}) \psi_{n-} (\gamma_{n+}q_{s+} - \gamma_{n-}q_{s-} + a\tilde{r}_s g),$$

$$T(a_+, t_s) - T(a_+, t_{s-1}) = \sum_{n=0}^N \Psi_{ns}(\tilde{\lambda}, \tilde{\zeta}) \psi_{n+} (\gamma_{n+} q_{s+} - \gamma_{n-} q_{s-} + a \tilde{r}_s g) .$$

The repeated application of this result generates the tridiagonal system of linear equations

$$\begin{bmatrix} A_s & -A_s^* & 0 & 0 \\ -\bar{A}_s^* & B_s & -B_s^* & 0 \\ 0 & -\bar{B}_s^* & \bar{B}_s & -A_s^* \\ 0 & 0 & -\bar{A}_s^* & \bar{A}_s \end{bmatrix} \begin{bmatrix} P_{s-} \\ p_{s-} \\ p_{s+} \\ P_{s+} \end{bmatrix} = ar_s \begin{bmatrix} 0 \\ 0 \\ \xi_s \\ -\bar{\xi}_s \end{bmatrix}$$

where the diagonal elements of the system matrix are

$$\begin{aligned} A_s &= \sum_{n=0}^N \Psi_{ns}(\lambda_h, \zeta_h) \psi_{n+} \gamma_{n+} + \sum_{n=0}^N \Psi_{ns}(\lambda_\delta, \zeta_\delta) \psi_{n-} \gamma_{n-} , \\ B_s &= \sum_{n=0}^N \Psi_{ns}(\lambda_\delta, \zeta_\delta) \psi_{n+} \gamma_{n+} + \sum_{n=0}^N \Psi_{ns}(\lambda, \zeta) \psi_{n-} \gamma_{n-} , \\ \bar{B}_s &= \sum_{n=0}^N \Psi_{ns}(\lambda_\delta, \zeta_\delta) \psi_{n-} \gamma_{n-} + \sum_{n=0}^N \Psi_{ns}(\lambda, \zeta) \psi_{n+} \gamma_{n+} , \\ \bar{A}_s &= \sum_{n=0}^N \Psi_{ns}(\lambda_h, \zeta_h) \psi_{n-} \gamma_{n-} + \sum_{n=0}^N \Psi_{ns}(\lambda_\delta, \zeta_\delta) \psi_{n+} \gamma_{n+} , \end{aligned}$$

the elements over its main diagonal are

$$A_s^* = \sum_{n=0}^N \Psi_{ns}(\lambda_\delta, \zeta_\delta) \psi_{n-} \gamma_{n+} , \quad B_s^* = \sum_{n=0}^N \Psi_{ns}(\lambda, \zeta) \psi_{n-} \gamma_{n+} ,$$

the elements under its main diagonal are

$$\bar{A}_s^* = \sum_{n=0}^N \Psi_{ns}(\lambda_\delta, \zeta_\delta) \psi_{n+} \gamma_{n-} , \quad \bar{B}_s^* = \sum_{n=0}^N \Psi_{ns}(\lambda, \zeta) \psi_{n+} \gamma_{n-}$$

and the right-hand side includes the elements

$$\xi_s = \sum_{n=0}^N \Psi_{ns}(\lambda_\delta, \zeta_\delta) \psi_{n-} g , \quad \bar{\xi}_s = \sum_{n=0}^N \Psi_{ns}(\lambda_\delta, \zeta_\delta) \psi_{n+} g .$$

We can see that, by means of the classical Gauss–Jacobi elimination, this system (divided by ar_s) can be decomposed to

$$\begin{bmatrix} A_s & -A_s^* & 0 & 0 \\ 0 & A_s B_s - A_s^* \bar{A}_s^* & -A_s B_s^* & 0 \\ 0 & -\bar{A}_s \bar{B}_s^* & \bar{A}_s \bar{B}_s - A_s^* \bar{A}_s^* & 0 \\ 0 & 0 & -\bar{A}_s^* & \bar{A}_s \end{bmatrix} \begin{bmatrix} \Theta_{s-} \\ \theta_{s-} \\ \theta_{s+} \\ \Theta_{s+} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \bar{A}_s^* \xi_s - A_s^* \bar{\xi}_s \\ -\bar{\xi}_s \end{bmatrix}$$

The solution of this system is given briefly by

$$\begin{aligned} C_s &= A_s B_s \bar{A}_s \bar{B}_s - A_s B_s A_s^* \bar{A}_s^* - A_s \bar{A}_s B_s^* \bar{B}_s^* - A_s^* \bar{A}_s^* \bar{A}_s \bar{B}_s + A_s^{*2} \bar{A}_s^{*2}, \\ \vartheta_{s-} &= A_s B_s^* (A_s^* \xi_s - \bar{A}_s \bar{\xi}_s) / C_s, \\ \vartheta_{s+} &= (A_s B_s - A_s^* \bar{A}_s^*) (A_s^* \xi_s - \bar{A}_s \bar{\xi}_s) / C_s; \end{aligned}$$

the evaluation of Θ_{s-} and Θ_{s+} is available, too, but is not necessary in our application. The complete formulae, applicable e. g. to formal differentiation (as compositions of functions) by λ and ζ , can be generated in the MATLAB code directly (they are rather long, although only $B_s, \bar{B}_s, B_s^*, \bar{B}_s^*$ and consequently C_s are really functions of λ and ζ , whereas $A_s, \bar{A}_s, A_s^*, \bar{A}_s^*, \xi_s$ and $\bar{\xi}_s$ are constants). However, we can conclude that for two special choices special $x \in \{-l, l\}$, substituting (7), we have obtained (8) in the form

$$\begin{aligned} T_N(-l, t_s) &= T_N(-l, t_{s-1}) \\ &\quad + \beta_-^T V \Psi_s(\lambda, \zeta) V^T M^{-1} (\beta_+ \vartheta_{s+}(\lambda, \zeta) - \beta_- \vartheta_{s-}(\lambda, \zeta) + ag) r_s, \\ T_N(l, t_s) &= T_N(l, t_{s-1}) \\ &\quad + \beta_+^T V \Psi_s(\lambda, \zeta) V^T M^{-1} (\beta_+ \vartheta_{s+}(\lambda, \zeta) - \beta_- \vartheta_{s-}(\lambda, \zeta) + ag) r_s. \end{aligned}$$

Its advantage is that both the vector function $\Psi_s(\lambda, \zeta)$ and two scalar functions $\vartheta_{s-}(\lambda, \zeta), \vartheta_{s+}(\lambda, \zeta)$ has been expressed explicitly yet.

5. OPTIMIZATION PROBLEM

The just derived explicit formulae for the evaluation of $T_N(-l, t_s)$ and $T_N(l, t_s)$ can be now compared with our data T_{s-}, T_{s+} . In the ideal case we should have

$$T_{s-} \approx T_N(-l, t_s), \quad T_{s+} \approx T_N(l, t_s).$$

Nevertheless, our physically realistic model has been simplified substantially, our practical calculations incorporate numerical errors (e. g. some finite numbers N and S are considered) and our imperfect equipment does not return exact values of temperature. Thus the existence of an exact solution of such system of $2S$ nonlinear equations with some λ and ζ cannot be expected in general.

Our aim is to set λ and ζ in the best way to minimize the errors in the preceding $2p$ equations. Let us consider the cost function

$$\Phi(\lambda, \zeta) = \frac{1}{2} \sum_{\sigma \in \{+, -\}} \sum_{s=1}^S (\Gamma_{s\sigma}(\lambda, \zeta))^2, \tag{9}$$

created from $2S$ components

$$\Gamma_{s\sigma}(\lambda, \zeta) = T_N(\sigma l, t_s) - T_{s\sigma}; \tag{10}$$

the symbol σ will denote the sign $+$ or $-$ everywhere. Various iterative approaches, based on the contraction principle and on the Banach fixed point theorem, are

available to seek for the best λ and ζ , minimizing (9). Since we can suppose that some practical (rather good) estimates of λ and ζ (e.g. for some similar materials from the table in [4], p. 28) are available, we are able to apply the Newton iterative method, using the recurrent corrections

$$\begin{bmatrix} \lambda \\ \zeta \end{bmatrix} \leftarrow \begin{bmatrix} \lambda \\ \zeta \end{bmatrix} - \begin{bmatrix} \partial^2\Phi/\partial\lambda^2 & \partial^2\Phi/\partial\lambda\partial\zeta \\ \partial^2\Phi/\partial\lambda\partial\zeta & \partial^2\Phi/\partial\zeta^2 \end{bmatrix}^{-1} \begin{bmatrix} \partial\Phi/\partial\lambda \\ \partial\Phi/\partial\zeta \end{bmatrix}. \quad (11)$$

To implement this algorithm in practice, we need to calculate all corresponding partial derivatives. In the rather compact form (sufficient for software development) we have for the first derivatives

$$\partial\Phi/\partial\lambda = \sum_{\sigma \in \{+, -\}} \sum_{s=1}^S \Gamma_{s\sigma} D_{s\sigma}^\lambda, \quad \partial\Phi/\partial\zeta = \sum_{\sigma \in \{+, -\}} \sum_{s=1}^S \Gamma_{s\sigma} D_{s\sigma}^\zeta \quad (12)$$

and for the second derivatives

$$\begin{aligned} \partial^2\Phi/\partial\lambda^2 &= \sum_{\sigma \in \{+, -\}} \sum_{s=1}^S ((D_{s\sigma}^\lambda)^2 + \Gamma_{s\sigma} D_{s\sigma}^{\lambda\lambda}), \\ \partial^2\Phi/\partial\zeta^2 &= \sum_{\sigma \in \{+, -\}} \sum_{s=1}^S ((D_{s\sigma}^\zeta)^2 + \Gamma_{s\sigma} D_{s\sigma}^{\zeta\zeta}), \\ \partial^2\Phi/\partial\lambda\partial\zeta &= \sum_{\sigma \in \{+, -\}} \sum_{s=1}^S (D_{s\sigma}^\lambda D_{s\sigma}^\zeta + \Gamma_{s\sigma} D_{s\sigma}^{\lambda\zeta}) \end{aligned}$$

where

$$\begin{aligned} D_{s\sigma}^\lambda &= \beta_\sigma^T V [\partial\Psi_s/\partial\lambda] V^T M^{-1} (\beta_+ \vartheta_{s+} - \beta_- \vartheta_{s-} + g) a r_s \\ &\quad + \beta_\sigma^T V \Psi_s (\beta_+ [\partial\vartheta_{s+}/\partial\lambda] - \beta_- [\partial\vartheta_{s-}/\partial\lambda]) a r_s, \\ D_{s\sigma}^\zeta &= \beta_\sigma^T V [\partial\Psi_s/\partial\zeta] V^T M^{-1} (\beta_+ \vartheta_{s+} - \beta_- \vartheta_{s-} + g) a r_s \\ &\quad + \beta_\sigma^T V \Psi_s (\beta_+ [\partial\vartheta_{s+}/\partial\zeta] - \beta_- [\partial\vartheta_{s-}/\partial\zeta]) a r_s, \\ D_{s\sigma}^{\lambda\lambda} &= \beta_\sigma^T V [\partial^2\Psi_s/\partial\lambda^2] V^T M^{-1} (\beta_+ \vartheta_{s+} - \beta_- \vartheta_{s-} + g) a r_s \\ &\quad + \beta_\sigma^T V \Psi_s (\beta_+ [\partial^2\vartheta_{s+}/\partial\lambda^2] - \beta_- [\partial^2\vartheta_{s-}/\partial\lambda^2]) a r_s, \\ D_{s\sigma}^{\zeta\zeta} &= \beta_\sigma^T V [\partial^2\Psi_s/\partial\zeta^2] V^T M^{-1} (\beta_+ \vartheta_{s+} - \beta_- \vartheta_{s-} + g) a r_s \\ &\quad + \beta_\sigma^T V \Psi_s (\beta_+ [\partial^2\vartheta_{s+}/\partial\zeta^2] - \beta_- [\partial^2\vartheta_{s-}/\partial\zeta^2]) a r_s, \\ D_{s\sigma}^{\lambda\zeta} &= \beta_\sigma^T V [\partial^2\Psi_s/\partial\lambda\partial\zeta] V^T M^{-1} (\beta_+ \vartheta_{s+} - \beta_- \vartheta_{s-} + g) a r_s \\ &\quad + \beta_\sigma^T V \Psi_s (\beta_+ [\partial^2\vartheta_{s+}/\partial\lambda\partial\zeta] - \beta_- [\partial^2\vartheta_{s-}/\partial\lambda\partial\zeta]) a r_s. \end{aligned}$$

The main difficulty is that the above sketched differentiation requires (in each step of the Newton method, improving the estimate of λ and ζ) rather complicated evaluation of first and second partial derivatives. Nevertheless, the resulting system consists only from two nonlinear algebraic equations; thus this approach promises to be much more effective than the 3-step ‘‘ad hoc’’ algorithm, usually applied by material engineers in such problems:

1. set some rough estimate of λ and ζ ,
2. using some (not very flexible) software package like ANSYS, calculate the distribution of T in time, including that in the measured points,
3. if the differences between the measured and calculated values of T are large (which is decided from experience), choose an other couple (λ, ζ) , using some heuristic access, and return to step 2, otherwise finish.

Moreover, we shall see that our approach supports also the probabilistic analysis of uncertainties in measurements, required by technical standards for the validation of setting of material characteristics; this should give better results than an imperfect “worst scenario” approach.

Although the convergence of the Newton method for practical calculations seems to be satisfactory, the problem of the convergence of this method (and of its quality) for the minimization of $\Phi(\lambda, \zeta)$ needs further investigations. The deeper convergence analysis should be based on some estimates for the Jacobian and Hessian of Φ , generated for a finite time interval with discrete measurements $\Gamma_{s\sigma}$. Let us also remark that the above mentioned ANSYS software is able to be used in another form, incorporating the design optimization (module /OPT); this may be seen as an alternative way for the effective solution of our inverse problem.

6. UNCERTAINTIES IN MEASUREMENT

One crucial duty in the procedure of certification of a laboratory, justifying its activity in some proposed professional scope, is to identify sources of uncertainties and quantify corresponding uncertainties in all its measurements. This may be rather hard and difficult (partially administrative) work, going beyond the research area of this article; for representative illustration we shall only assume that uncertainties in our measurement may be connected purely with the uncorrelated quantities r_s (adjusted), $s \in \{1, \dots, p\}$, and T_{s+} and T_{s-} , $s \in \{1, \dots, S\}$ (measured by sensors).

We have derived two implicit formulae, coming from two conditions $\partial\Phi/\partial\lambda = \partial\Phi/\partial\zeta = 0$ (needed for the minimization of (9)), for the evaluation of λ and ζ . This offers the possibility to use standard approaches of mathematical statistics to guarantee the comprehension of “true values” of real constants λ and ζ to some two-dimensional domain in a real plane with certain probability. Such access, highly recommended by [5], p. 25 (with references to technical standards), has been applied e. g. in [2] to the calculation of incident radiation from the total heat flux gauge measurements. In our measurement let w_r and w_T be the uncertainties of variables r and T_s (the same for any s). Then the classical results from mathematical statistics and probabilistic theory, namely the central limit theorem (discussed e. g. in the textbook [16], p. 111, properly) justify the analysis of uncertainties with help of normal (Gaussian) probability distributions, characterized by their mean values and standard deviations. Consequently the uncertainties w_λ and w_ζ of variables λ and ζ can be expressed (following [2], p. 609) in the form

$$w_\lambda = \sqrt{w_r^2 \sum_{s=1}^S (\partial\lambda/\partial r_s)^2 + w_T^2 \sum_{\sigma \in \{+, -\}} \sum_{s=1}^S (\partial\lambda/\partial T_{s\sigma})^2},$$

$$w_\zeta = \sqrt{w_r^2 \sum_{s=1}^S (\partial\zeta/\partial r_s)^2 + w_T^2 \sum_{\sigma \in \{+, -\}} \sum_{s=1}^S (\partial\zeta/\partial T_{s\sigma})^2}.$$

To evaluate w_λ and w_ζ seems now to be very easy: it is sufficient to calculate $\partial\lambda/\partial v$ and $\partial\zeta/\partial v$ for each $v \in \{r_1, \dots, r_s, T_{1-}, \dots, T_{S-}, \dots, T_{1+}, \dots, T_{S+}\}$. However, one difficulty occurs: we do not know λ and ζ from explicit formulae, thus we must get these partial derivatives (in the statistics well-known as “sensitivity coefficients”) from the system of two linear algebraic equations

$$\begin{bmatrix} \partial^2\Phi/\partial\lambda^2 & \partial^2\Phi/\partial\lambda\partial\zeta \\ \partial^2\Phi/\partial\lambda\partial\zeta & \partial^2\Phi/\partial\zeta^2 \end{bmatrix} \cdot \begin{bmatrix} \partial\lambda/\partial v \\ \partial\zeta/\partial v \end{bmatrix} + \begin{bmatrix} \partial(\partial\Phi/\partial\lambda)/\partial v \\ \partial(\partial\Phi/\partial\zeta)/\partial v \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix},$$

whose solution is

$$\begin{bmatrix} \partial\lambda/\partial v \\ \partial\zeta/\partial v \end{bmatrix} = - \begin{bmatrix} \partial^2\Phi/\partial\lambda^2 & \partial^2\Phi/\partial\lambda\partial\zeta \\ \partial^2\Phi/\partial\lambda\partial\zeta & \partial^2\Phi/\partial\zeta^2 \end{bmatrix}^{-1} \begin{bmatrix} \partial(\partial\Phi/\partial\lambda)/\partial v \\ \partial(\partial\Phi/\partial\zeta)/\partial v \end{bmatrix}.$$

Let us notice that the same matrix inversion requirement occurs in the algorithm (11).

In both equations (12) $T_{s\sigma}$ (for any $s \in \{1, \dots, S\}$ and $\sigma \in \{+, -\}$) is hidden, thanks to (10), only as an additive term in $\Gamma_{s\sigma}$, thus $\partial\Gamma_{s\sigma}/\partial T_{s\sigma} = -1$. This yields

$$\partial(\partial\Phi/\partial\lambda)/\partial T_{s\sigma} = - \sum_{\sigma \in \{+, -\}} \sum_{s=1}^S D_{s\sigma}^\lambda, \quad \partial(\partial\Phi/\partial\zeta)/\partial T_{s\sigma} = - \sum_{\sigma \in \{+, -\}} \sum_{s=1}^S D_{s\sigma}^\zeta.$$

In the analogous way we can see that r_s is contained in $\Gamma_{s\sigma}$ as a multiplicative term; therefore

$$\begin{aligned} \partial(\partial\Phi/\partial\lambda)/\partial r_s &= \sum_{\sigma \in \{+, -\}} \sum_{s=1}^S \beta_\sigma^T V \Psi_s V^T M^{-1} (\beta_+ \vartheta_{s+} - \beta_- \vartheta_{s-}) D_{s\sigma}^\lambda \\ &+ \sum_{\sigma \in \{+, -\}} \sum_{s=1}^S \beta_\sigma^T V [\partial\Psi_s/\partial\lambda] V^T M^{-1} (\beta_+ \vartheta_{s+} - \beta_- \vartheta_{s-} + g) a, \\ \partial(\partial\Phi/\partial\zeta)/\partial r_s &= \sum_{\sigma \in \{+, -\}} \sum_{s=1}^S \beta_\sigma^T V \Psi_s V^T M^{-1} (\beta_+ \vartheta_{s+} - \beta_- \vartheta_{s-}) D_{s\sigma}^\zeta \\ &+ \sum_{\sigma \in \{+, -\}} \sum_{s=1}^S \beta_\sigma^T V [\partial\Psi_s/\partial\zeta] V^T M^{-1} (\beta_+ \vartheta_{s+} - \beta_- \vartheta_{s-} + g) a. \end{aligned}$$

The set of uncertain quantities can be naturally extended: e.g. by particular times t_s , lengths l , h and δ , etc. One can see that namely some uncertainty of l (the size of our tested material sample) should be taken into consideration: the MATLAB-supported derivation of $\partial(\partial\Phi/\partial\lambda)/\partial l$ and $\partial(\partial\Phi/\partial\zeta)/\partial l$ makes use of the same arguments as those of $T_{s\sigma}$ and r_s , but the results are formally more complicated and less reader-friendly.

7. CONCLUSION AND APPLICATION

We have demonstrated how the basic thermal technical characteristics λ and $c = \zeta/\rho$ for the heat transfer equation (1) can be identified, using a relatively cheap both measurement equipment and computational technique. In this way the analogy of the table from [4], p.28, can be composed for a large class of building materials, including those with a complicated porous structure, sensitive to moisture influence; e. g. some new ecological materials for insulation layers, exploiting the wood waste – the design of such advanced materials is one of the research activities at the Faculty of Civil Engineering of the Brno University of Technology.

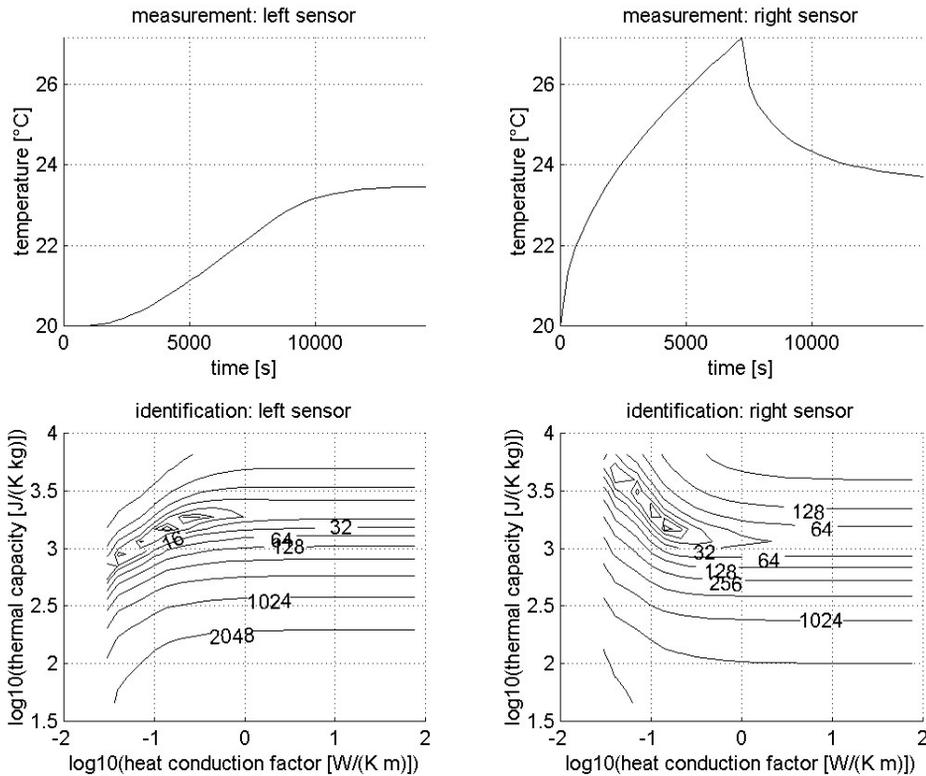


Fig. Time development of two measured temperatures.

Let us introduce a new insulation material, based on small wood particles, bound by the silicate paste; $\rho = 650 \text{ kg/m}^3$, $T_0 = 20 \text{ }^\circ\text{C}$, $S = 48$, $\tau_1 = \dots = \tau_S = 300 \text{ s}$. The experiment is arranged in the following way: the right-hand aluminium plate produces the energy output 33333 W/m^3 during $24 \times 300 = 7200 \text{ s}$, then the system is getting cold during 7200s again; for $\delta = 1 \text{ mm}$, $l = 50 \text{ mm}$ and $h = 200 \text{ mm}$ this corresponds to $r(t) = 33.333 \text{ W/m}^3$ for $t \leq 7200 \text{ s}$ and to zero $r(t)$ for $t > 7200 \text{ s}$. We know that $\lambda_\delta = 204 \text{ W/(K m)}$, $\rho_\delta = 2600 \text{ kg/m}^3$, $c_\delta = 440 \text{ J/(K kg)}$, $\zeta_\delta = \rho_\delta c_\delta$, $\lambda_h =$

0.04 W/(K m), $\rho_h = 45 \text{ kg/m}^3$, $c_h = 1550 \text{ J/(K kg)}$ and $\zeta_h = \rho_h c_h$. All quantities on the figure are presented in SI physical units, the temperature in °C. The upper part of the figure shows the time development of the temperature T for $x = -l$ and for $x = l$, obtained experimentally for $s \in \{1, \dots, S\}$. The cost function $\Phi \text{ [K}^2\text{]}$ from (9) consists of two additive parts: of Φ_- and of Φ_+ , according to the sign σ in the first sum. Although this is not needed in our algorithm, for illustration in the lower part of the figure we present the distribution of Φ_- (the left-hand part) and of Φ_+ (the right-hand part) for various values of λ (the horizontal axis) and $c = \zeta/\rho$ (the vertical axis); the isolines are drawn for powers of 2, 21² discrete values of λ and ζ were considered, both axes are labeled in the common logarithm scale. We can observe that Φ_+ and Φ_- are not sensitive to λ and to c in the same way; however, the linearized theory of the heat transfer (including our numerical analysis) seems to be valid with rather high precision, as $\Phi = \Phi_- + \Phi_+$ is close to zero for “optimal values” $\lambda = 0.15 \text{ W/(K m)}$ and $c = 1550 \text{ J/(K kg)}$. The analysis of uncertainties in such measurement needs the reliable estimate of w_r and w_T ; this should be obtained by more comparative measurements, making use of materials with a priori known values of λ and $\zeta = \rho c$.

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