Least-squares based technique for identification of thermal characteristics of building materials

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***Abstract*—**The thermomechanical behavior of building materials and whole engineering structures is conditioned by their complicated non-periodic microstructure and non-deterministic influences from external environment, involving phase changes, moisture transport, etc. However, technical standards require evaluation of effective (macroscopic) material characteristics for simplified linear differential or integral equations. Even if related direct mathematical and computational problems (with a priori known material characteristics) are rather easy, inverse problems (with missing or uncertain values of some material characteristics) may be ill-posed and non-stable, requiring artificial regularization. This article demonstrates how to avoid some difficulties of this type in the case of identification of basic thermal characteristics, namely of the thermal conductivity and of the heat capacity (including the potential effect of interface heat transfer), using the numerical least squares technique. The corresponding laboratory equipment, supplied by the robust MATLAB-based computational tool, is presented.

***Keywords*—**Building materials, inverse problems, heat transfer, least squares method, partial differential equations of evolution.

I. Introduction

The reliable prediction of behavior of building structures and their parts is a serious and complicated problem, involving, in addition to their static and dynamic behavior under various mechanical loads, also their thermal behavior, conditioned by the thermal technical properties of all used materials. Advanced building materials for both constructive and insulation layers have typically a porous structure, admitting gas and liquid flows (cf. [6]), perhaps even phase changes, namely those utilizing the latent heat of special materials to better thermal performance and stability of building objects by [20], or those occurring during the controlled treatment of early-age silicate composites, preventing volume changes that initiate micro- and macrofracturing, e.g. of maturing concrete mixtures and similar silicate composites by [25].

The proper analysis of corresponding physical (and related chemical) processes leads to the formulation of complicated initial and boundary value problems, generated by the macro-scale balance laws of classical thermomechanics: of mass, of (linear and angular) momentum and of energy (or enthalpy), including all available microstructural data. Although many open problems still occur both in the existence and regularity of solutions of such problems and in the convergence of their finite-dimensional approximations (cf. [8]), effective and reliable computational algorithms are required from the engineering practice. However, their quality is conditioned by the reasonable design and setting of material characteristics, often also functions of unknown non-stationary variables, coming from algebraic or differential constitutive relations.

We shall pay attention namely to the experimental identification of basic thermal technical characteristics, i.e. the thermal conductivity λ and the heat capacity c (related to a volume unit): by most European technical standards λ measures the insulation ability of material, c its accumulation ability; alternatively $\kappa = \rho\, c$ (the heat capacity related to a mass unit) may be considered where ρ denotes the material density. The stationary or indirect measurements give often bad or uncertain results just in the case of advanced building materials, e.g. those developed at the Faculty of Civil Engineering of Brno University of Technology (BUT); thus some new methodology of experimental work is needed. Various attempts (as so-called frequency-domain method, step-heating method, hot-strip / hot-wire method, infra-red photography approach, etc.) are documented in [2] and [9].

The rather simple, non-expensive and non-destructive measurement equipment, designed in the Laboratory of Building Physics of BUT, whose basic idea has been explained in [22], is based on the carefully controlled generation of heat fluxes into the practically closed measurement system and on the recording of temperature development in time. This equipment needs non-trivial computational support for the reconstruction of λ and κ from the overdetermined initial and boundary evolutionary problem; however, such inverse mathematical problems, as discussed in [13], p. 20, are typically ill-posed and non-stable and require artificial regularization.

The approach presented in [21] for a one-dimensional simplification, based on the modified Fourier method and on the eigenvalue analysis by [3], p. 175, is rather complicated and does not admit simple extension to the 2- and 3-dimensional cases. The alternative approach of [23] demonstrates how such difficulties can be overcome, thanks to a special class of measurement configurations, using only non-homogenous Dirichlet boundary conditions, applying the finite element method with Hermite polynomials as basis functions (to guarantee the optimal precision both for the temperature and for all heat fluxes) for the discretization in the space variable x and the Crank–Nicholson scheme in the time variable t. Consequently the least squares optimization, compatible with [5], p. 367, is applied; an overview of alternative optimization approaches for inverse problems of heat transfer, as deterministic, evolutionary, stochastic, hybrid, etc., can be found in [7]. The computational algorithm of [23], coming from the

Newton iterative method, has been implemented in the MATLAB environment. This paper shows how such approach, exceeding the classification [1], can be generalized naturally to the 2- and 3-dimensional measurement configurations, more realistic in the laboratory practice, including the effect of heat transfer at non-perfect material interfaces.

II. Evolution equations

Let us consider the following measurement configuration: a specimen, located in some open set Ω_1 in the three-dimensional Euclidean space, is inserted between two metal (e.g. aluminum) plates, in an union of two open sets Ω_2, surrounded by the thick (e.g. polystyrene) insulation, in an open set Ω_3. For simplicity, we shall assume that all mentioned sets are domains with sufficiently smooth boundaries, preserving all standard results of the theory of Lebesgue and Sobolev spaces, namely the trace theorem, Sobolev imbedding theorems and Green-Ostrogradskii theorem, in sense of [11] and [18]. Fig. 1 shows such geometrical configuration, suitable for laboratory measurements. Another geometrical configuration, better for measurements in situ, e.g. of massive concrete structures, is sketched at Fig. 2.

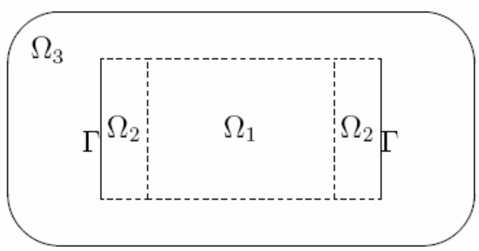

Fig. 1 Basic measurement configuration

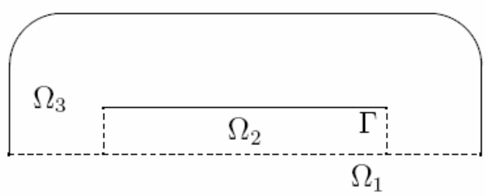

Fig. 2 Modified measurement configuration

Assuming that the temperature τ_e of external environment is constant and that the initial temperature of all parts of the measurement system is equal to τ_e, we are able to study the time development of temperature τ in the measurement system, i.e. on all domains Ω_i with $i \in \{1,2,3\}$, in the Cartesian coordinate system $x = (x_1, x_2, x_3)$ in the three-dimensional Euclidean space for any time $t \in I$; the dot symbol for the derivatives with respect to t will be used. Only Ω_3 has the external boundary, denoted by Ω_{3e} and supplied by the local outward normal unit vector $\nu = (\nu_1, \nu_2, \nu_3)$; similar vector can be introduced on all interfaces Γ_{ij} between Ω_i and Ω_j with $(i,j) \in \{(1,2),(1,3),(2,3)\}$, preserving orientation from Ω_i to Ω_j.

The evolution of the temperature τ on Ω_1, Ω_2 and Ω_3 and also of the heat flux q on Γ_{12}, Γ_{13}, Γ_{23} and Γ_{3e}, is driven by the controlled generation of the additional heat flux q_* from $W^{1,2}(I, L^2(\Gamma_{23}))$ (non-zero only on a suitable part of Γ_{23} in practice). We will assume that such evolution can be described by the linearized non-stationary equations of heat conduction on Ω_1, Ω_2 and Ω_3, characterized by λ and κ, and that the heat transfer between all these domains and between Ω_3 and the external environment are characterized by the heat transfer coefficient α, taking λ and κ as constants on each Ω_i with $i \in \{1,2,3\}$ and α as a constant on each Γ_{ij} with $(i,j) \in J := \{(1,2),(1,3),(2,3),(3,e)\}$. However, the values of λ and κ on Ω_1 and the values of α on Γ_{12} and Γ_{13} (4 values totally, corresponding to a tested specimen), unlike the values of of λ and κ on Ω_2 and Ω_3 and the values of α on Γ_{23} and Γ_{3e}, are a priori unknown; this missing information is compensated by recording the temperature difference $u_* \in L^\infty(I, L^2(\Gamma))$ (in practice: its discrete values), related to τ_e, on $\Gamma_{23} \times I$ where Γ is some part of Γ_{23}: one could expect that u_* coincides with

$$u := \tau - \tau_e$$

there.

Let us introduce the notations $(.,.)_i$ for scalar products in $L^2(\Omega_i)$ and in $L^2(\Omega_i)^3$ with arbitrary $i \in \{1,2,3\}$, $(.,.)_{ij}$ for scalar products in $L^2(\Gamma_{ij})$ with arbitrary $(i,j) \in J$ and

$$B_i(v,w) := (v, \kappa \dot{w})_i + (\nabla v, \lambda \nabla w)_i$$

for any $v \in V$ and $w \in L^2(I,V)$ with arbitrary $i \in \{1,2,3\}$. In addition to the standard notation of Lebesgue and Sobolev spaces and other (abstract) function spaces, compatible with [11] and [18], for the sake of brevity we shall use also

$$H := L^2(\Omega_1) \times L^2(\Omega_2) \times L^2(\Omega_3),$$
$$X := L^2(\Gamma_{12}) \times L^2(\Gamma_{13}) \times L^2(\Gamma_{23}) \times L^2(\Gamma_{3e}),$$
$$W_*^{1,2}(\Omega_3) := \{w \in W^{1,2}(\Omega_3) : w = 0 \text{ on } \Gamma_{3e}\},$$
$$V := W^{1,2}(\Omega_1) \times W^{1,2}(\Omega_2) \times W_*^{1,2}(\Omega_3).$$

Our problem is now to find such $u \in L^\infty(I,V) \cap C(I,H)$ with $\dot{u} \in L^\infty(I,H)$ and such $q \in L^\infty(I,X)$ that for any $v \in V$ and $p \in P$

$$\begin{aligned}
B_1(v,u) + (v,q)_{12} + (v,q)_{13} &= 0, \\
B_2(v,u) - (v,q)_{12} + (v,q)_{23} &= 0, \\
B_3(v,u) - (v,q)_{13} - (v,q)_{23} + (v,q)_{3e} &= (v,q_*)_{23}, \\
(p,u^{(1)})_{12} - (p,u^{(2)})_{12} + (p,\alpha q)_{12} &= 0, \\
(p,u^{(1)})_{13} - (p,u^{(3)})_{13} + (p,\alpha q)_{13} &= 0, \\
(p,u^{(2)})_{23} - (p,u^{(3)})_{23} + (p,\alpha q)_{23} &= -\tfrac{1}{2}(p,\alpha q_*)_{23}, \\
(p,u^{(3)})_{3e} + (p,\alpha q)_{3e} &= 0
\end{aligned} \tag{1}$$

holds where $u^{(i)}$ with $i \in \{1,2,3\}$ refer to traces of u from Ω_i; the evident discontinuity of q on Γ_{23} is handled (to avoid artificial jumps in function values like [15]) taking $q + q_*$ instead of q on Γ_{23} for the heat flux into Ω_3. The integral formulation of the system of partial differential equations of evolution (1) can be converted into the classical (differential) one (at least in sense of distributions), using the Green-Ostrogradskii theorem (on the integration by parts): introducing

$$\mathcal{B}u := \kappa\dot{u} - \lambda\Delta u \ ,$$
$$\mathcal{L}u := \lambda\nabla u\cdot\nu \ ,$$

thanks to the piecewise constant values of λ, we receive

$$\begin{aligned}
(v,\mathcal{B}u)_1 + (v,\mathcal{L}u+q)_{12} + (v,\mathcal{L}u+q)_{13} &= 0 \ ,\\
(v,\mathcal{B}u)_2 + (v,\mathcal{L}u-q)_{12} + (v,\mathcal{L}u+q)_{23} &= 0 \ ,\\
(v,\mathcal{B}u)_3 - (v,\mathcal{L}u-q)_{13} + (v,\mathcal{L}u-\tilde{q})_{23} + (v,\mathcal{L}u-q)_{3e} &= 0 \ ,\\
(p,u^{(1)})_{12} - (p,u^{(2)})_{12} + (p,\alpha q)_{12} &= 0\\
(p,u^{(1)})_{13} - (p,u^{(3)})_{13} + (p,\alpha q)_{13} &= 0 \ ,\\
(p,u^{(2)})_{23} - (p,u^{(3)})_{23} + (p,\alpha q + \tfrac{1}{2}\alpha\tilde{q})_{23} &= 0 \ ,\\
(p,u^{(3)})_{3e} + (p,\alpha q)_{3e} &= 0
\end{aligned}$$

where $\tilde{q} := q + q_*$. Consequently

$$\begin{aligned}
\kappa\dot{u} &= \lambda\Delta u && \text{on } \Omega_i \text{ with } i\in\{1,2,3\},\\
\lambda\nabla u^{(i)}\cdot\nu + q &= 0 && \text{on } \Gamma_{ij} \text{ with } (i,j)\in\Theta,\\
\lambda\nabla u^{(j)}\cdot\nu - q &= 0 && \text{on } \Gamma_{ij} \text{ with } (i,j)\in\Theta,\\
\lambda\nabla u^{(2)}\cdot\nu + q &= 0 && \text{on } \Gamma_{23},\\
\lambda\nabla u^{(3)}\cdot\nu - q &= q_* && \text{on } \Gamma_{23},\\
u^{(i)} - u^{(j)} + \alpha q &= 0 && \text{on } \Gamma_{ij} \text{ with } (i,j)\in\Theta,\\
u^{(2)} - u^{(3)} + \tfrac{1}{2}\alpha q &= -\tfrac{1}{2}\alpha q_* && \text{on } \Gamma_{ij} \text{ with } (i,j)\in\Theta,\\
u^{(3)} + \alpha q &= 0 && \text{on } \Gamma_{3e} \ .
\end{aligned}$$

Clearly the first line here represents the heat transfer equation, coming from the thermodynamic law of energy conservation, implementing the Fourier constitutive law, on particular sets Ω_1, Ω_2 and Ω_3, the second, third, fourth and fifth lines refer to corresponding boundary conditions in terms of interface heat fluxes and all remaining lines express interface temperature jumps using such fluxes. Most experimental settings try to minimize the effect of interface temperature jumps: for perfect contacts between Ω_1, Ω_2 and Ω_3 everywhere we can set $\alpha\to\infty$, which forces the interface temperature continuity. This can be done for α on Γ_{3e}, too, but heat fluxes to external environment are usually negligible (at least for t_* sufficiently small) because of the thick insulation in Ω_3.

III. Convergence of Rothe sequences

Assuming that all material characteristics λ, κ and α are positive and prescribed everywhere, we are able, to derive the solution of (1) , thanks to the linearity of (1), using the method of discretization in time. Such approach, incorporating also available information from microstructure, using the two-scale convergence technique, is discussed in details in [24] where relevant references (missing here) can be found, too.

For an integer m let us construct the Rothe sequences $u^m\in L^\infty(I,V)$, $\bar{u}^m\in L^\infty(I,V)$ and $\bar{q}^m\in L^\infty(I,X)$, defined (as the image of a corresponding abstract function, i.e. for any admissible x) as

$$\begin{aligned}
u^m(t) &:= u^m_{s-1} + (t/h - s + 1)(u^m_s - u^m_{s-1}) \ ,\\
\bar{u}^m(t) &:= u^m_s \ ,\\
\bar{q}^m(t) &:= q^m_s \ ,
\end{aligned}$$

using the Euler explicit scheme, for any $(s-1)h < t \le sh$, $h = t_*/m$ and $s\in\{1,\dots,m\}$, $u^m_0 := 0$ and $q^m_0 := 0$ everywhere, and insert them formally as $\dot{u}\approx\dot{u}^m$, $u\approx\bar{u}^m$ and $q\approx\bar{q}^m$ into (1). Instead of q_* we are able to take $\bar{q}^m_*(t)$, introduced, apparently in the best way, as the mean value q^m_{*s} of the time integral of q_* from $(s-1)h$ to sh for every $s\in\{1,\dots,m\}$. However, the more simple choice

$$\bar{q}^m_*(t) := q^m_{*s} := q_*(sh)$$

is sufficient: we have

$$\int_I |\,q^m_*(t) - q_*(t)\,|\,\mathrm{d}t = \sum_{s=1}^{m}\int_{(s-1)h}^{sh} |\,q_*(sh) - q_*(t)\,|\,\mathrm{d}t$$
$$= \sum_{s=1}^{m}\int_{(s-1)h}^{sh} |\int_t^{sh}\dot{q}_*(\zeta)\ \mathrm{d}\zeta\,|\,\mathrm{d}t \le h\sum_{s=1}^{m}\int_{(s-1)h}^{sh}|\,\dot{q}_*(\zeta)\,|\,\mathrm{d}\zeta = h\int_I |\,\dot{q}_*(\zeta)\,|\,\mathrm{d}\zeta \ ,$$

thus (for formal zero values of q_* outside Γ_{23})

$$\bar{q}^m_* \text{ converges strongly to } q_* \text{ in } L^\infty(I,X),$$

etc. Our aim is to derive analogous convergence results for (a priori unknown) sequences u^m, $\bar{u}^m$ and $\bar{q}^m$; we will do this in 3 steps.

The first step verifies the solvability of the time-discretized system of partial differential equations in an arbitrary s-th time step. Omitting all upper indices m if no risk of misunderstanding occurs, from (1) we obtain

$$\begin{aligned}
&(v,\kappa\hat{u}_s)_1 + (\nabla v,\lambda\nabla u_s)_1\\
&\quad + (v,q_s)_{12} + (v,q_s)_{13} &&= 0 \ ,\\
&(v,\kappa\hat{u}_s)_2 + (\nabla v,\lambda\nabla u_s)_2\\
&\quad - (v,\hat{q}_s)_{12} + (v,\hat{q}_s)_{23} &&= 0 \ ,\\
&(v,\kappa\hat{u}_s)_3 + (\nabla v,\lambda\nabla u_s)_3\\
&\quad - (v,q_s)_{13} - (v,q_s)_{23} + (v,q_s)_{3e} &&= (v,q_{*s})_{23} \ ,\\
&(p,u^{(1)}_s)_{12} - (p,u^{(2)}_s)_{12} + (p,\alpha q_s)_{12} &&= 0 \ ,\\
&(p,u^{(1)}_s)_{13} - (p,u^{(3)}_s)_{13} + (p,\alpha q_s)_{13} &&= 0 \ ,\\
&(p,u^{(2)}_s)_{23} - (p,u^{(3)}_s)_{23} + (p,\alpha q_s)_{23} &&= -\tfrac{1}{2}(p,\alpha q_{*s})_{23} \ ,\\
&(p,u^{(3)}_s)_{3e} + (p,\alpha q_s)_{3e} &&= 0 \ .
\end{aligned} \tag{2}$$

where

$$\hat{u}_s := (u_s - u_{s-1})/h \,;$$

later also

$$\hat{q}_s := (q_s - q_{s-1})/h \ ,$$
$$q_{*s} := (q_{*s} - q_{*s-1})/h$$

will be needed. Thanks to the linearity of $(u_s,q_s)\in V\times X$ in (2), the Lax-Milgram theorem (discussed in great details in [19]) guarantees the existence and uniqueness of (u_s,q_s) in $V\times X$ if the bilinear form

$$h^{-1}\sum_{i=1}^{3}(v,\kappa v)_i + \sum_{i=1}^{3}(\nabla v,\lambda\nabla v)_i + \sum_{(i,j)\in J}(p,\alpha p)_{ij} - 2\sum_{(i,j)\in J}(v^{(i)}-v^{(j)},p)_{ij}$$

for any $(v,p)\in V\times X$ admits a lower estimate

$$\chi(\|v\|^2+\|\nabla v\|^2+\|p\|_\times^2)$$

where $\|.\|$ is the standard norm in H or in $H\times H\times H$, $\|.\|_\times$ the standard norm in X and χ some positive constant. However, the Cauchy-Schwarz inequality (cf. [11], p. 77) together with the trace theorem (whose detailed analysis can be found in [18], p. 211) yield the estimates

$$\begin{aligned} 2(v^{(l)},p)_{ij} &\le \omega\|v\|_\times^2 + \omega^{-1}\|p\|_\times^2 \\ &\le k\omega\varepsilon^{-1}\|v\|^2 + \omega\varepsilon\|\nabla v\|^2 + \omega^{-1}\|p\|_\times^2 \end{aligned} \tag{3}$$

with $(i,j)\in J$, $l\in\{i,j\}$ except e, certain positive constant k (from the trace theorem) and arbitrary positive constants ω and ε. Therefore the verification of existence of some constant χ requires only a sufficiently small time step h.

Applying special choices of (v,p) in (1) and (2), the second step brings useful a priori estimates of u^m, $\bar{u}^m$ and $\bar{q}^m$. In addition to (2), we need also the difference between 2 systems (2), formulated in the s-th and $s-1$-th time steps, divided by h, for $s>1$, i.e.

$$\begin{aligned} h^{-1}(v,\kappa(\hat{u}_s-\hat{u}_{s-1}))_1+(\nabla v,\lambda\nabla\hat{u}_s)_1 \\ +(v,\hat{q}_s)_{12}+(v,\hat{q}_s)_{13} &= 0\,, \\ h^{-1}(v,\kappa(\hat{u}_s-\hat{u}_{s-1}))_2+(\nabla v,\lambda\nabla\hat{u}_s)_2 \\ -(v,\hat{q}_s)_{12}+(v,\hat{q}_s)_{23} &= 0\,, \\ h^{-1}(v,\kappa(\hat{u}_s-\hat{u}_{s-1}))_3+(\nabla v,\lambda\nabla\hat{u}_s)_3 \\ -(v,\hat{q}_s)_{13}-(v,\hat{q}_s)_{23}+(v,\hat{q}_s)_{3e} &= (v,\hat{q}_{*s})_{23}\,, \\ (p,\hat{u}_s^{(1)})_{12}-(p,\hat{u}_s^{(2)})_{12}+(p,\alpha\hat{q}_s)_{12} &= 0\,, \\ (p,\hat{u}_s^{(1)})_{13}-(p,\hat{u}_s^{(3)})_{13}+(p,\alpha\hat{q}_s)_{13} &= 0\,, \\ (p,\hat{u}_s^{(2)})_{23}-(p,\hat{u}_s^{(3)})_{23}+(p,\alpha\hat{q}_s)_{23} &= -\tfrac{1}{2}(p,\alpha\hat{q}_{*s})_{23}\,, \\ (p,\hat{u}_s^{(3)})_{3e}+(p,\alpha\hat{q}_s)_{3e} &= 0\,. \end{aligned} \tag{4}$$

Let us notice that both (u_s,q_s) and $(\hat{u}_s,\hat{q}_s)$ belong to $V\times X$, thus we can set in particular $(v,p)=(u_s,q_s)$ in (2), as well as $(v,p)=h^{-1}(\hat{u}_s,\hat{q}_s)$ in (4). The first of these settings gives

$$\begin{aligned} (u_s,\kappa\hat{u}_s)_1+(\nabla u_s,\lambda\nabla u_s)_1 \\ +(u_s^{(1)},q_s)_{12}+(u_s^{(1)},q_s)_{13} &= 0\,, \\ (u_s,\kappa\hat{u}_s)_2+(\nabla u_s,\lambda\nabla u_s)_2 \\ -(u_s^{(2)},q_s)_{12}+(u_s^{(2)},q_s)_{23} &= 0\,, \\ (u_s,\kappa\hat{u}_s)_3+(\nabla u_s,\lambda\nabla u_s)_3 \\ -(u_s^{(3)},q_s)_{13}-(u_s^{(3)},q_s)_{23}+(u_s^{(3)},q_s)_{3e} &= (u_s,q_{*s})_{23}\,, \\ (q_s,u_s^{(1)})_{12}-(q_s,u_s^{(2)})_{12}+(q_s,\alpha q_s)_{12} &= 0\,, \\ (q_s,u_s^{(1)})_{13}-(q_s,u_s^{(3)})_{13}+(q_s,\alpha q_s)_{13} &= 0\,, \\ (q_s,u_s^{(2)})_{23}-(q_s,u_s^{(3)})_{23}+(q_s,\alpha q_s)_{23} &= -\tfrac{1}{2}(q_s,\alpha q_{*s})_{23}\,, \\ (q_s,u_s^{(3)})_{3e}+(q_s,\alpha q_s)_{3e} &= 0\,, \end{aligned} \tag{5}$$

the second one similarly

$$\begin{aligned} h^{-1}(\hat{u}_s,\kappa(\hat{u}_s-\hat{u}_{s-1}))_1+(\nabla\hat{u}_s,\lambda\nabla\hat{u}_s)_1 \\ +(\hat{u}_s^{(1)},\hat{q}_s)_{12}+(\hat{u}_s^{(1)},\hat{q}_s)_{13} &= 0\,, \\ h^{-1}(\hat{u}_s,\kappa(\hat{u}_s-\hat{u}_{s-1}))_2+(\nabla\hat{u}_s,\lambda\nabla\hat{u}_s)_2 \\ -(\hat{u}_s^{(2)},\hat{q}_s)_{12}+(\hat{u}_s^{(2)},\hat{q}_s)_{23} &= 0\,, \\ h^{-1}(\hat{u}_s,\kappa(\hat{u}_s-\hat{u}_{s-1}))_3+(\nabla\hat{u}_s,\lambda\nabla\hat{u}_s)_3 \\ -(\hat{u}_s^{(3)},\hat{q}_s)_{13}-(\hat{u}_s^{(3)},\hat{q}_s)_{23}+(\hat{u}_s^{(3)},\hat{q}_s)_{3e} &= (\hat{u}_s,\hat{q}_{*s})_{23}\,, \\ (\hat{q}_s,\hat{u}_s^{(1)})_{12}-(\hat{q}_s,\hat{u}_s^{(2)})_{12}+(\hat{q}_s,\alpha\hat{q}_s)_{12} &= 0\,, \\ (\hat{q}_s,\hat{u}_s^{(1)})_{13}-(\hat{q}_s,\hat{u}_s^{(3)})_{13}+(\hat{q}_s,\alpha\hat{q}_s)_{13} &= 0\,, \\ (\hat{q}_s,\hat{u}_s^{(2)})_{23}-(q_s,\hat{u}_s^{(3)})_{23}+(\hat{q}_s,\alpha\hat{q}_s)_{23} &= -\tfrac{1}{2}(\hat{q}_s,\alpha\hat{q}_{*s})_{23}\,, \\ (\hat{q}_s,\hat{u}_s^{(3)})_{3e}+(\hat{q}_s,\alpha\hat{q}_s)_{3e} &= 0\,. \end{aligned} \tag{6}$$

Applying the obvious identity

$$2\sum_{i=1}^{3}(u_s,u_s-u_{s-1})_i = \|u_s\|^2-\|u_{s-1}\|^2+\|u_s-u_{s-1}\|^2$$

and, analogously to (3), with the same indexes and constants k, ω and ε, the estimates

$$\begin{aligned} 2h(u_s^{(l)},q_s)_{ij} &\le \omega h\|u_s\|_\times^2 + \omega^{-1}h\|q_s\|_\times^2 \\ &\le k\omega\varepsilon^{-1}h\|u_s\|^2 + \omega\varepsilon h\|\nabla u_s\|^2 + \omega^{-1}h\|q_s\|_\times^2 \end{aligned}$$

true also for q_s replaced by q_{*s}, as well as

$$2h(q_s,q_{*s})_{23} \le \omega h\|q_s\|_\times^2 + \omega^{-1}h\|q_{*s}\|_\times^2\,,$$

summing up all equations (5) with $s\in\{1,...,r\}$ for any $r\in\{1,...,m\}$, for appropriate choice of ω and ε we come to the estimate

$$\begin{aligned} &\|u_r\|^2 + h\sum_{s=1}^{r}\|\nabla u_s\|^2 + h\sum_{s=1}^{r}\|q_s\|_\times^2 \\ &\le \varpi h\sum_{s=1}^{r}\|u_s\|^2 + \varpi h\sum_{s=1}^{r}\|q_{*s}\|_\times^2\,, \end{aligned} \tag{7}$$

containing certain positive constant ϖ. Since

$$\sqrt{h\sum_{s=1}^{r}\|q_{*s}\|_\times^2}$$

is just the norm of the bounded sequence $\bar{q}_*^m$ in $L^2(I,X)$, the discrete version of the Gronwall lemma (see [16]) then yields that

$\bar{u}^m(t)$ is bounded in H for each $t\in I$,

$\bar{u}^m$ is bounded in $L^2(I,V)$,

$\bar{q}^m$ is bounded in $L^2(I,X)$.

Unfortunately, this is not sufficient for the complete convergence analysis, as announced. Nevertheless, summing up similarly all equations (6) with $s\in\{2,...,r\}$, we come to the estimate

$$\begin{aligned} &\|\hat{u}_r\|^2 + h^{-1}\sum_{s=1}^{r}\|\nabla u_s-\nabla u_{s-1}\|^2 + h^{-1}\sum_{s=1}^{r}\|q_s-q_{s-1}\|_\times^2 \\ &\le \varpi h\sum_{s=1}^{r}\|\hat{u}_s\|^2 + \varpi h^{-1}\sum_{s=1}^{r}\|q_{*s}-q_{*s-1}\|_\times^2 + \|\hat{u}_1\|^2\,; \end{aligned} \tag{8}$$

moreover we have

$$\|\nabla u_r\|^2 \le (\sum_{s=1}^{r}\|\nabla u_s - \nabla u_{s-1}\|)^2 \le r\sum_{s=1}^{r}\|\nabla u_s - \nabla u_{s-1}\|^2$$

$$\le t_* h^{-1}\sum_{s=1}^{r}\|\nabla u_s - \nabla u_{s-1}\|^2$$

and also

$$h^{-1}\sum_{s=1}^{r}\| q_{*s} - q_{*s-1}\|_\times = h^{-1}\sum_{s=1}^{r}\|\int_{(s-1)h}^{sh}\dot{q}_*(t)\ \mathrm{d}t\|_\times$$

$$\le \sum_{s=1}^{r}\int_{(s-1)h}^{sh}\|\dot{q}_*(t)\|_\times\ \mathrm{d}t \le \int_I \|\dot{q}_*(t)\|_\times\ \mathrm{d}t\ .$$

For the right side of (8) it remains to estimate

$$\|\hat{u}_1\|^2 = h^{-2}\|u_1\|^2 .$$

In particular (7) with $r=1$ implies

$$(1-\varpi h)\|u_1\|^2 \le \varpi h \|q_{*1}\|_\times^2\ .$$

But

$$\|q_{*1}\|_\times = \|\int_0^h \dot{q}(t)\ \mathrm{d}t\|_\times \le h \sup_{0\le t\le h}\|\dot{q}(t)\|_\times ;$$

this forces the boundedness of $\|\hat{u}_1\|$ for sufficiently small h.

The discrete version of the Gronwall lemma (again) yields that

$\bar{u}^m(t)$ is bounded in V for each $t\in I$,

$\bar{q}^m(t)$ is bounded in V for each $t\in I$,

$\dot{u}^m$ is bounded in H for each $t\in I$.

The third step is to find the limits of u^m, $\bar{u}^m$ and $\bar{q}^m$ and identify them with the solution (u,q) of (1). The Eberlein-Shmul'yan theorem (see [11], p. 197) together with the Sobolev imbedding theorem (see [11], p. 134) guarantee (up to subsequences) that

$\bar{u}^m$ converges weakly to some u in $L^\infty(I,V)$,

$\bar{q}^m$ converges weakly to some q in $L^\infty(I,X)$,

$\dot{u}^m$ converges strongly to some $\hat{u}$ in $L^\infty(I,H)$.

It is easy to see that $\hat{u}$ (whose time integral belongs is a continuous abstract function mapping I to H) coincides with $\dot{u}$: assuming

$$\|u(t)-\int_0^t u(\zeta)\ \mathrm{d}\zeta\| \ne 0 \text{ for some } t\in I ,$$

we obtain the contrary

$$\|u(t)-\int_0^t u(\zeta)\ \mathrm{d}\zeta\| = \lim_{m\to\infty}\|\bar{u}^m(t)-u^m(t)\|$$

$$= \lim_{m\to\infty}\|h\dot{u}^m(t)\| = 0\ .$$

Consequently, the limit passage from (2) to (1) is available.

The same approach can be applied to the verification of uniqueness of the above constructed solution (u,q) of (1). Let us consider another solution $(\breve{u},\breve{q})$ satisfying (1) and introduce

$$\bar{u} = u-\breve{u}\ ,$$

$$\bar{q} = q-\breve{q}\ .$$

The difference between both versions of (1) with $v=\bar{u}$ and $p=\bar{q}$ degenerates to

$$\begin{aligned}
B_1(\bar{u},\bar{u}) + (\bar{u},\bar{q})_{12} + (\bar{u},\bar{q})_{13} &= 0\ ,\\
B_2(\bar{u},\bar{u}) - (\bar{u},q)_{12} + (\bar{u},q)_{23} &= 0\ ,\\
B_3(\bar{u},\bar{u}) - (\bar{u},\bar{q})_{13} - (\bar{u},\bar{q})_{23} + (\bar{u},\bar{q})_{3e} &= 0\ ,\\
(\bar{q},\bar{u}^{(1)})_{12} - (\bar{q},\bar{u}^{(2)})_{12} + (\bar{q},\alpha\bar{q})_{12} &= 0\ ,'\\
(\bar{q},\bar{u}^{(1)})_{13} - (\bar{q},\bar{u}^{(3)})_{13} + (\bar{q},\alpha\bar{q})_{13} &= 0\ ,\\
(\bar{q},\bar{u}^{(2)})_{23} - (\bar{q},\bar{u}^{(3)})_{23} + (\bar{q},\alpha\bar{q})_{23} &= 0\ ,\\
(\bar{q},\bar{u}^{(3)})_{3e} + (\bar{q},\alpha\bar{q})_{3e} &= 0\ .
\end{aligned}$$

Since

$$\int_0^t B_i(\bar{u}(\zeta),\bar{u}(\zeta))\ \mathrm{d}\zeta = \tfrac{1}{2}(\bar{u}(t),\kappa\bar{u}(t))_i$$

for any $i\in\{1,2,3\}$ and arbitrary $t\in I$, we receive finally the estimate

$$\|\bar{u}(t)\|^2 + \int_0^t\|\nabla\bar{u}(\varsigma)\|^2\ \mathrm{d}\zeta + \int_0^t\|\bar{q}(\varsigma)\|_\times^2\ \mathrm{d}\zeta \le \varpi\int_0^t\|\bar{u}(\varsigma)\|^2\ \mathrm{d}\zeta\ .$$

The classical (continuous) Gronwall lemma (see [16]) then guarantees zero values of both $\bar{u}$ and $\bar{q}$, thus $u=\breve{u}$ and $q=\breve{q}$.

Let us notice that the slightly generalized definition of the Rothe sequences

$$u^m(t) := u^m_{s-1} + (t/h-s+1)(u^m_s - u^m_{s-1})\ ,$$

$$\bar{u}^m(t) := (1-\xi)u^m_{s-1} + \xi u^m_s\ ,$$

$$\bar{q}^m(t) := (1-\xi)q^m_{s-1} + \xi q^m_s\ ,$$

leads, repeating all above sketched arguments, to the same qualitative convergence results with $\frac{1}{2}\le\xi\le 1$, especially both for the Euler implicit scheme $\xi=1$ (not for the Euler explicit scheme $\xi=0$) and for the Crank-Nicholson scheme with $\xi=\frac{1}{2}$; the technical details can be left to the reader. In the following section we will utilize just the Crank-Nicholson scheme.

IV. Discrete approximation

In our measurement system the information on λ, κ and α is incomplete: only $\lambda=\lambda_i$, $\kappa=\kappa_i$ with $i\in\{2,3\}$ are given constants on Ω_i and α_{ij} with $(i,j)\in\{(2,3),(3,e)\}$ are given constants on Ω_{ij}, whereas $\lambda=\lambda_1$ and $\kappa=\kappa_1$ remains to be identified on Ω_i and the same is true for α_{ij} with $(i,j)\in\{(1,2),(1,3)\}$, i.e. for all material characteristics related to the tested specimen. Inserting some estimates of λ_1, κ_1, α_{12} and α_{13} into (1), we are able to obtain corresponding (u,q), probably not satisfying the condition $u=u_*$ in $L^\infty(I,L^2(\Gamma))$. Unfortunately, to satisfy it exactly in impossible because of presence of errors from various sources:

i) errors coming from the assumptions of linearized model of heat conduction (material homogeneity and isotropy, negligible effect of other physical processes, as moisture propagation, contaminant transport, heat convection and radiation, etc.),

ii) errors of the hardware and software imperfections, both of the measurement and the computational devices,
iii) errors of the computational algorithm (effects of x - and t -discretization, later also of inaccurate optimization),
iv) errors in all data q_* and u_*.

However, we can make the sensitivity analysis of the influence of setting λ_1, κ_1, α_{12} and α_{13} to the approximate validity of $u = u_*$.

In the following formulas (where λ_i and κ_i with $i \in \{2,3\}$ and α_{ij} with $(i,j) \in \{(2,3),(3,e)\}$ are nod needed explicitly) all indexes in λ_1, κ_1, α_{12} and α_{13} will be omitted for brevity; to prevent the mismatch, we shall write α instead of α_{12} and β instead of α_{13}. The complete numerical simulation of experiments needs the full discretization, both in t and in x; the appropriate choice of a numerical technique is the finite element approximation with Hermite basis, taking into account nodal parameters ϑ as discrete values of $(u, \nabla u)$ and η as-discrete values of q for any time step $t = sh$ with some $s \in \{1,...,m\}$ and for fixed λ, κ, α and β we receive only a system of linear algebraic equation with a sparse symmetrical real system matrix.

The general form of such system, step-by-step for $s \in \{1,...,m\}$, applying the Crank-Nicholson scheme, is

$$2h^{-1}(\lambda M + N)(\vartheta_s - \vartheta_{s-1}) + (\kappa K + L)(\vartheta_s + \vartheta_{s-1}) + S(\eta_s + \eta_{s-1}) = f_s + f_{s-1},$$

$$S^T(\vartheta_s + \vartheta_{s-1}) + (\alpha P + \beta Q + R)(\eta_s + \eta_{s-1}) = g_s + g_{s-1}$$

where M, N, K, L, P, Q, R, S are real matrices, containing λ_i and κ_i with $i \in \{2,3\}$ and α_{ij} with $(i,j) \in \{(2,3),(3,e)\}$; the elements K and L (due to the approximation of ∇u and ∇v using Hermite functions with small compact support) involve moreover the multiplicative factor $1/\delta^2$ where δ represents the typical edge length in the regular family of finite element decomposition, $f_0,...,f_m$ and $g_0,...,g_m$ are certain real vectors. From the physical and engineering point of view, the left-hand side matrices express the material characteristics, the right-hand side vectors represent the controlled artificial heat flux. Introducing the notation

$$A := \kappa K + L + 2h^{-1}(\lambda M + N),$$
$$B := \kappa K + L - 2h^{-1}(\lambda M + N),$$
$$C := \alpha P + \beta Q + R,$$
$$\varphi_s := (f_{s-1} + f_s)/2,$$
$$\psi_s := (g_{s-1} + g_s)/2,$$

we have

$$\begin{bmatrix} A & S \\ S^T & C \end{bmatrix} \cdot \begin{bmatrix} \vartheta_s \\ \eta_s \end{bmatrix} = \begin{bmatrix} \varphi_s \\ \psi_s \end{bmatrix} - \begin{bmatrix} B & S \\ S^T & C \end{bmatrix} \cdot \begin{bmatrix} \vartheta_{s-1} \\ \eta_{s-1} \end{bmatrix}. \tag{9}$$

Since A, B, C in (9) are linear matrix functions of parameters $\lambda, \kappa, \alpha, \beta$, their derivatives are $A_{,\lambda} = -B_{,\lambda} = 2h^{-1}M$, $A_{,\kappa} = B_{,\kappa} = K$, $C_{,\alpha} = P$ and $C_{,\beta} = Q$. For any parameter $\varsigma \in \{\lambda, \kappa, \alpha, \beta\}$ we obtain

$$\begin{bmatrix} A & S \\ S^T & C \end{bmatrix} \cdot \begin{bmatrix} \vartheta_{s,\varsigma} \\ \eta_{s,\varsigma} \end{bmatrix} = \begin{bmatrix} \varphi_{s\varsigma} \\ \psi_{s\varsigma} \end{bmatrix} - \begin{bmatrix} B & S \\ S^T & C \end{bmatrix} \cdot \begin{bmatrix} \vartheta_{s-1,\varsigma} \\ \eta_{s-1,\varsigma} \end{bmatrix}$$

for the first derivatives of ϑ_s and η_s and

$$\begin{bmatrix} A & S \\ S^T & C \end{bmatrix} \cdot \begin{bmatrix} \vartheta_{s,\varsigma\varsigma} \\ \eta_{s,\varsigma\varsigma} \end{bmatrix} = 2\begin{bmatrix} \varphi_{s\varsigma} \\ \psi_{s\varsigma} \end{bmatrix} - \begin{bmatrix} B & S \\ S^T & C \end{bmatrix} \cdot \begin{bmatrix} \vartheta_{s-1,\varsigma\varsigma} \\ \eta_{s-1,\varsigma\varsigma} \end{bmatrix}$$

for all non-zero second ones where

$$\varphi_{s\lambda} := -2h^{-1}M(\vartheta_s - \vartheta_{s-1}),\ \varphi_{s\kappa} := -K(\vartheta_{s-1} + \vartheta_s),$$
$$\psi_{s\alpha} := -P(\eta_{s-1} + \eta_s),\ \psi_{s\beta} := -Q(\eta_{s-1} + \eta_s)$$

and all remaining terms $\varphi_{s\varsigma}$ and $\psi_{s\varsigma}$ with $\varsigma \in \{\lambda, \kappa, \alpha, \beta\}$ are zero vectors; in particular for $s = 1$ all derivatives of ϑ_{s-1} and η_{s-1} vanish.

V. Least-squares identification

The aim of the identification procedure is to find such parameters λ and κ (which cannot be usually done quite without α and β, although their role should be reduced under laboratory conditions) that minimize some appropriate error function F. In our experimental configuration it is natural to choose

$$F = \tfrac{1}{2}\langle u - u_*,\ u - u_* \rangle \tag{10}$$

where $\langle .,. \rangle$ denotes the scalar product (more generally: a symmetrical bilinear form) in $L^2(I, L^2(\Gamma))$; further generalizations of this least-squares approach, still other than taking $L^\gamma(I, L^2(\Gamma))$ with $2 \le \gamma \le \infty$ instead of $L^2(I, L^2(\Gamma))$, will be discussed later. In practice we are able to construct the reasonable finite-dimensional approximation of u, using ϑ_s with $s \in \{1,...,m\}$; the corresponding limit passage $h \to 0$ and $\delta \to 0$ is available. Let us notice that F is a real function of 4 variables only; the effective algorithm seeking for $(\lambda, \kappa, \alpha, \beta)$ can be then based on the classical Newton iterative procedure

$$\tilde{\varsigma} = \varsigma - F_{,\varsigma}/F_{,\varsigma\varsigma}$$

where $\tilde{\varsigma}$ is an improved value of $\varsigma \in \{\lambda, \kappa, \alpha, \beta\}$ and

$$F_{,\varsigma} = \langle u_{,\varsigma}, u - u_* \rangle,$$
$$F_{,\varsigma\varsigma} = \langle u_{,\varsigma\varsigma}, u - u_* \rangle + \langle u_{,\varsigma}, u_{,\varsigma} \rangle,$$

applied to an admissible closed set $(\lambda, \kappa, \alpha, \beta)$, including no negative values.

An alternative approach makes use of measured data u_* in the system of evolution equation of type (1). However, to have just $v \in V$ again, we need, instead of $\tau = u + \tau_e$, another decomposition $\tau = u + \tau_\times \in W^{1,2}(\Omega_1) \times W^{1,2}(\Omega_2) \times W_*^{1,2}(\Omega_3)$ (not unique in general) with $\tau_\times = \tau_e$ on Γ_{3e} and $\tau_\times = \tau_e + u_*$ on Γ; this brings some technical complications to (1). The heat flux q_* on Γ_{23} may be substituted by $q_\times := \lambda \nabla(\tau_\times + u^{(3)}) - q$, sufficiently on such $\Gamma_\times \subseteq \Gamma_{23}$ where $q_* \ne 0$. Consequently (9) (with substantially modified matrices and vectors) needs no formal changes, but the reasonable form of (10) is

$$F = \tfrac{1}{2}\left\langle q + q_* - \lambda\nabla(\tau_\times + u^{(3)}),\ q + q_* - \lambda\nabla(\tau_\times + u^{(3)})\right\rangle; \quad (11)$$

outside $\Gamma_\times$ all contributions to F are zero. A mixed approach using the weighted least-squares formulation of F is possible, too; the motivation for such computational experiments may come from the different accuracy and reliability of values q_* and u_*.

The computational algorithm offers the possibility of quick evaluation of changes of identified parameters forced by the modified input data. However, the general approach is able to consider the variables (u,q) also as functions of parameters θ from the sample space Ξ of elementary events; such sample space must be supplied by the minimal σ-algebra on Ξ and by certain probability measure $\mathcal{P}$. Then it is possible to replace F in (6) e.g. by

$$F = \tfrac{1}{2}\int_{\Xi}\left\langle u(\theta) - u_*(\theta),\ u(\theta) - u_*(\theta)\right\rangle \,\mathrm{d}\mathcal{P}$$

and apply some uncertainty representation technique, as the Karhunen-Loève or polynomial chaos expansions by [28], p.10, [12] and [14], or, alternatively, a Bayesian approach by [28], p. 25, and [17], compatible with [10], p. 26.

VI. Laboratory equipment

The discussed algorithm has been implemented in the original computational software (still in progress), supporting the measurements in the Laboratory of Building Physics of BUT. All functions are written in MATLAB; no additional software packages are needed. The example demonstrates the algorithm robustness, even under strong theoretical simplifications and non-precise measurements.

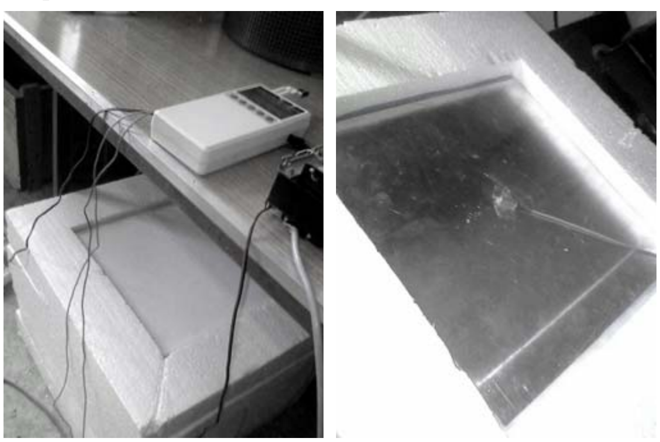

Fig. 3 Measurement equipment in the Laboratory of Building Physics at BUT (left photo), detail of heated plate (right photo).

Fig. 3 shows the complete laboratory measurement system, corresponding to the geometrical scheme at Fig. 1, and its crucial component – one of two aluminum plates; only one of them is heated there. Fig. 4 presents all particular measurement layers; to make it possible, some polystyrene insulation blocks are missing.

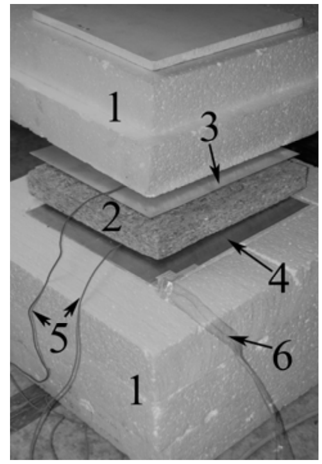

Fig. 4 Equipment components: 1 polystyrene insulation Ω_3, 2 material specimen Ω_1, 3 and 4 two aluminum plates Ω_2 (3 heated, 4 non-heated), 5 wiring to temperature sensors, 6 wiring to heating.

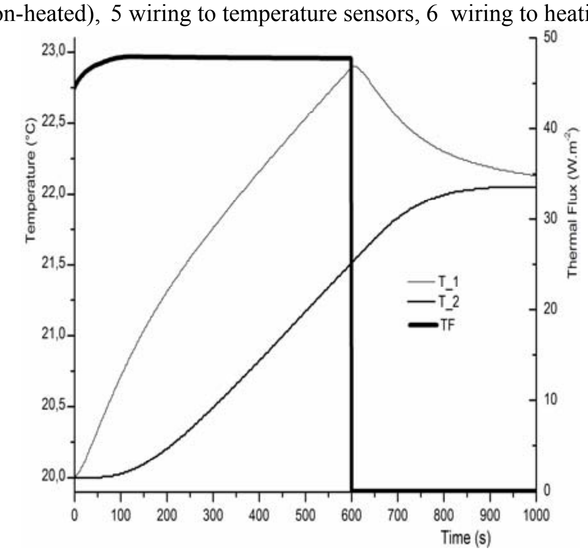

Fig. 5 Measured temperature $\tau_e + u_*$ [°C] on heated plate (T_1) and non-heated plate (T_2), generated thermal flux q_* [W/m^2] (TF), both from 0 to 1000 s, heating from 0 to 600 s.

The process of our MATLAB-supported experimental identification of parameters λ and κ on Ω_1 for an experimental porous concrete specimen assumes that all factors $1/\alpha$ are negligible in the whole system and reducible to one-dimensional problem of heat conduction in the perpendicular direction of x_1 to 6 parallel planes (3 couples) Γ_{12}, Γ_{23} and Γ_{3e}. Fig. 5 shows the generated heat flux in the time interval I from 0 to 1000 s, non-zero from 0 to 600 s, and the measured temperature on both aluminum / polystyrene interfaces. Fig. 6 presents the resulting distribution of temperature τ along x_1 in selected time steps, temperature gradient $\mathrm{d}\tau/\mathrm{d}x_1$ (all remaining components of $\nabla\tau$ are neglected) and heat flux $-\lambda\,\mathrm{d}\tau/\mathrm{d}x_1$ (with different λ on particular layers).

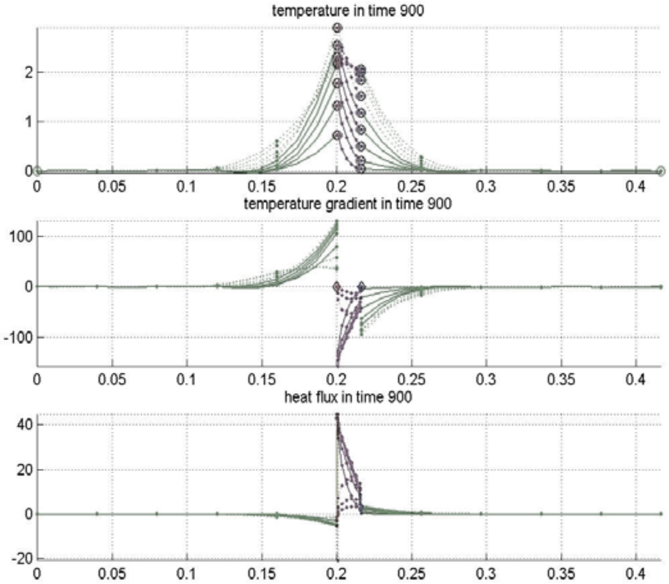

Fig. 6 Least-squares optimized time development of temperature [°C], temperature gradient [K/m] and heat flux [W/m^2] (full curves up to 600 s, dotted otherwise), horizontal axis x_1 [m].

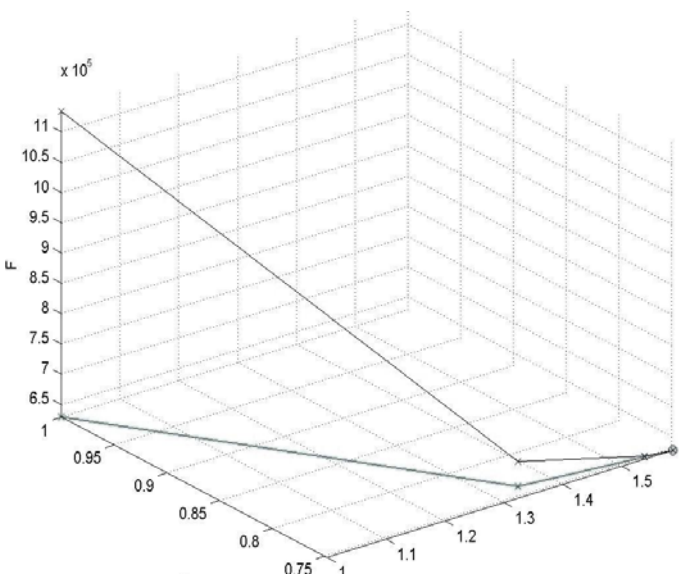

Fig. 7 Newton iterative procedure: $a = a_0 w_a$ [m^2/s] with $a_0 = 3.4\ 10^{-7}$ m^2/s, $b = b_0 w_b$ with $b_0 = 3.5$ Km/W, right horizontal axis shows w_a [-], left one w_b [-], F [(K/m)^2] is evaluated by (11), multiplied by b_0.

The transformed parameters $a = \lambda / \kappa$ and $b = 1/\lambda$ were considered; the computational advantages of such transformation in one-dimensional simplification are explained in [15]. Fig. 7 documents the convergence of the Newton iterative algorithm; error F was calculated as in (5), multiplied by the first estimate of λ.

VII. Conclusions

We have demonstrated the development of the inexpensive and robust measurement device, based on the non-trivial mathematical analysis of the direct and inverse theory of heat transfer problems. Even the identification procedure documented on Fig. 5, 6 and 7 figures, applying strong simplifications, seems to produce reasonable results.

More complex experimental configurations, demonstrating the relation of this work to the large research project AdMaS (Advanced Materials, Structures and Technologies), starting in January 2011 at BUT, will be presented in [26]. However, most presented results need further generalization in several directions: analysis of anisotropic materials, effect of heat convection and radiation, coupling with other physical processes, proper uncertainty analysis, etc. This can be taken as the motivation for further research, whose aim is to derive comparable results for a much larger class of material characteristics in engineering applications of classical thermodynamics, namely to the processes mentioned in *Introduction*.

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