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COMPUTATIONAL OPTIMIZATION OF MATERIAL CHOICE FOR THERMAL CONTAINERS OF ADVANCED BUILDINGS

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Abstract. Optimization of performance of thermal containers installed in advanced buildings stimulates the multidisciplinary research, covering civil and mechanical engineering studies, material testing and physical, mathematical and computational analysis, up to the implementation of algorithms. This paper pays attention namely to the hot-wire identification of thermal characteristics of materials, with references to more general optimization tools.

Keywords: heat transfer, building design, inverse and optimization problems

Mathematics subject classification: Primary 35K05; Secondary 74A15, 35K10, 65K10

1 Introduction

Decreasing amount of energy sources, together with new achievement in the design of advanced materials, structures and technologies, stimulates the multidisciplinary research coupling civil and mechanical engineering studies, material testing and physical, mathematical and computational analysis. The European directive [2] forces the passive energy standard, whose proper formulation comes from [1], for both new and reconstructed buildings since 2020. One promising way for substantial reduction of energy requirements of buildings, namely those with controlled interior temperature, is connected with the design and construction of high-temperature thermal containers.

A representative example of such research activities seems to be the collaboration of the Brno University of Technology, Faculty of Civil Engineering (FCE BUT), with the Swedish specialists in fibre-optics-based heat production systems and with the Czech firm Alumistr a. s. Hrušovany (20 km southern from Brno), supported by the Technological Agency of the Czech Republic 2012–15. Apart from the successful construction and performance of a model house, supplied by the massive silicate thermal container, with no requirements to external energy sources, this project brings a strong motivation for further research in optimized choice of materials for thermal containers in the first step, followed by more general optimization of design of relevant structures and equipments. Since the technical details of the project solutions are not available for free access yet, the illustrative Fig. 1 shows just the first small model of the thermal container and documents one of the first series of high-temperature experiments with material specimens intended for the real container, namely for the evaluation of their basic thermal technical characteristics.

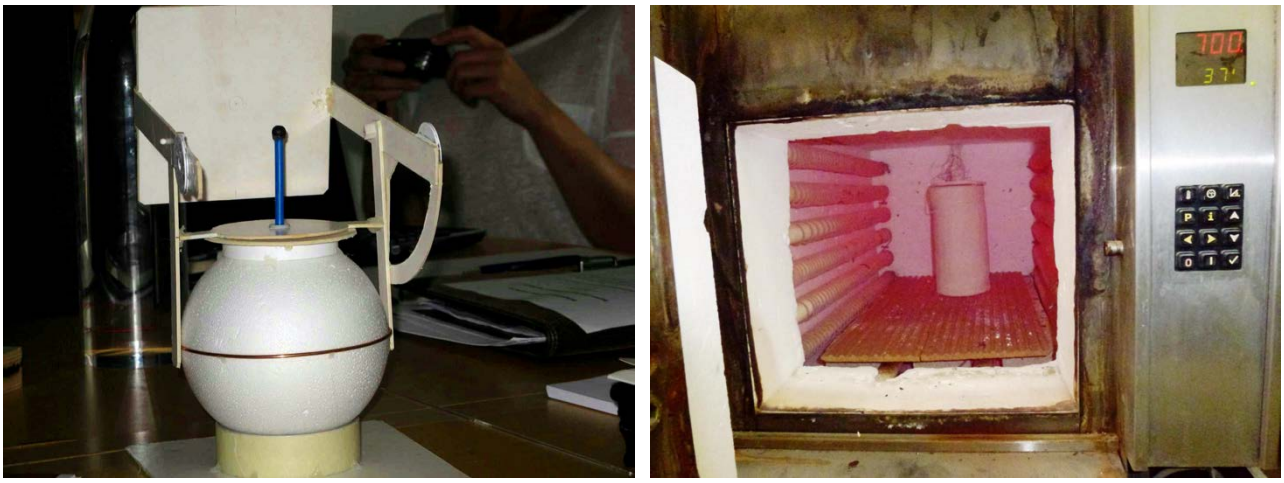

Fig. 1. A small model of thermal container (left photo). A cylindrical silicate specimen in the laboratory oven at the temperature 700 °C (right photo).

Much more consideration related to thermal collection and storage can be found in [4]. Practical equipments make use of i) sensible heat of high-temperature resistant materials by [5], or ii) materials involving phase-change components, appropriate for intended temperature levels, as parafine capsules, by [6]. In this paper we shall pay attention to i) with selected silicate materials, compatible with [7], namely to the computational evaluation of their thermal conductivity and diffusivity, as a substantial information for the reasonable design of the heat container; this will be supported by the hot-wire experimental setting, generalizing the approach of the European standard [8].

As a model problem for our physical, mathematical and computational analysis, we shall start with the study of of pure thermal conduction in an (at least macroscopically) isotropic medium without internal heat sources. However, the dependence of material characteristics on the temperature cannot be neglected, as usual in the case of temperature near to 20 °C, prescribed for building interiors – cf. [9]. This brings serious difficulties to the analysis of corresponding both direct and inverse problems, as well as to the relevant experiment planning.

2 A direct problem

Proper formulation of thermal processes starts with the conservation principles of selected scalar quantities, as for mass, (linear and angular) momentum and energy, from classical thermomechanics. Here, for simplicity, we shall work only with the conservation of thermal energy, with the absolute Kelvin temperature $\theta(x,t)$ as the reference variable. Here $x = (x_1, x_2, x_3)$ refers to the Cartesian coordinate system in the Euclidean space R^3, whereas t denotes the time from some interval $I = [0,T]$, assuming a finite positive T.

Let Ω be an open set (typically a domain) in R^3 with its boundary $\partial\Omega$ where the (formally outward) unit normal vector $\nu(x) = (\nu_1(x), \nu_2(x), \nu_3(x))$ can be introduced almost everywhere (which needs certain smoothness assumption – cf. [11], p. 16). We shall use upper dots instead of $\partial/\partial t$ for brevity, as well as Hamilton operators $\nabla = (\partial/\partial x_1, \partial/\partial x_2, \partial/\partial x_3)$ and central dots for scalar products in R^3. Consequently we can write e. g. Laplace operators briefly as $\Delta = \partial^2/\partial x_1^2 + \partial^2/\partial x_2^2 + \partial^2/\partial x_3^2 = \nabla\cdot\nabla$.

Following [10], p. 5, the classical formulation of energy conservation reads

$$\dot{\varepsilon} + \nabla \cdot q = 0 \qquad \text{on } \Omega \times I \tag{1}$$

where ε [J/m^3] represents the thermal energy (per unit volume) and $q = (q_1, q_2, q_3)$ the thermal flux [W/m^2]. Clearly (1) must be supplied by appropriate empirical constitutive equations coupling ε and q with θ. Here we shall suppose

$$\dot{\varepsilon} = \kappa\dot{\theta}\,, \qquad q = -\lambda\nabla\theta \qquad \text{on } \Omega \times I\,, \tag{2}$$

with two positive-valued material characteristics λ and κ: λ [W/(m.K)] is well-known as the thermal conductivity, κ [J/(m^3.K)] as the thermal capacity per unit volume; frequently the thermal capacity c [J/(kg.K)] is considered instead of κ, with the evident relation $\kappa = c\rho$ where ρ is the material density [kg/m^3] (evaluable from simple experiments in most cases). Let us notice that we are allowed to assume λ and κ independent of t (unlike x) directly, but their dependence on $\theta(x,t)$ may be substantial.

For simplicity, we shall consider only the Cauchy initial condition

$$\theta(.,0) = \theta_0 \qquad \text{on } \Omega \tag{3}$$

and the Neumann boundary one

$$q \cdot \nu = q_* \qquad \text{on } \partial\Omega \times I\,; \tag{4}$$

θ_0 must be prescribed on Ω and q_* on $\partial\Omega \times I$. Inserting (2) into (1), we have

$$\kappa\dot{\theta} - \nabla \cdot (\lambda\nabla\theta) = 0 \qquad \text{on } \Omega \times I\,, \tag{5}$$

and exploiting (2), too, similarly

$$-\lambda\nabla\theta \cdot \nu = q_* \qquad \text{on } \partial\Omega \times I\,. \tag{6}$$

Moreover, the thermal diffusivity α [m^2/s] is also introduced in many papers, alternatively to κ or c. The motivation is clear: for homogeneous materials, i. e. with constant λ and κ, taking $\alpha = \lambda/\kappa$, we can rewrite (5) to

$$\dot{\theta} - \alpha\Delta\theta = 0 \qquad \text{on } \Omega \times I\,. \tag{7}$$

However, to derive the analogy of (7) for inhomogeneous materials is not easy; this requires the application of the both enthalpy and Kirchhoff transforms by [11], pp. 68, 253, 291. Moreover, even for homogeneous materials, λ in (6) cannot be replaced by α (which does not allow the separate evaluation of α later in an inverse problem).

For numerical evaluation of θ, at least for all cases where no sufficiently simple forms of analytical solutions are available, the weak formulation of (5), (3) and (6) is useful. Using the standard notation of Lebesque, Sobolev, Bochner, etc. (abstract) function spaces, compatible with [11], pp. 10, 15, 23, and $(.,.)$ for scalar products in both $L^2(\Omega)$ and $L^2(\Omega)^3$ (Lebesgue intergals) and $\langle .,. \rangle$ for scalar products in $L^2(\partial\Omega)$ (Hausdorff integrals), we can write (5) and (6) in the integral form

$$(v, \kappa\dot{\theta}) + (\nabla v, \lambda\nabla\theta) = \langle v, q_* \rangle \qquad \text{on } I \tag{8}$$

for every test function $v \in W^{1,2}(\Omega)$; (3) remains to be consider separately. It is natural to assume $\theta_0 \in W^{1,2}(\Omega)$ and, at least for $\lambda, \kappa \in L^\infty(\Omega)$, moreover $q_* \in L^2(\partial\Omega)$. Consequently, for the linear parabolic system of evolution (8), using the convergence results for Rothe sequences by [11], p. 202, the existence and uniqueness of $\theta \in L^2(I, W^{1,2}(\Omega)$ with $\dot{\theta} \in L^2(I, L^2(\Omega)$ can be verified without

difficulties. However, this is not true for λ and κ dependent of θ where additional growth conditions are necessary; for more details see [12], with numerous references to [11] (namely on the available results for quasilinear equations of evolution) again.

Let us remark that (5) and (6) can be derived from (8) using the Green-Ostrogradskiĭ theorem, at least in the distributional sense. However, this does not guarantee any regularity (which may be needed in applications), as discussed in [11], p. 215.

In particular, for constant λ and κ, various special (even classical) solutions of (5) can be found in the literature; they differs in the reasonable applicability of (6) for special geometrical configurations, often using numerical techniques again, as boundary elements on $\partial\Omega$ instead of finite elements on Ω. In this paper we shall utilize the following result of [13]:

$$\theta = \theta_0 + \frac{Q}{4\pi\lambda}\,\mathrm{Ei}\left(\frac{r^2}{4\alpha t}\right)\,, \tag{9}$$

including the exponential integral

$$\mathrm{Ei}(\varsigma) = \int_{\varsigma}^{\infty} \frac{\exp(v)}{v}\,\mathrm{d}v = -\gamma - \ln\varsigma + \varsigma + \epsilon(\varsigma)\,, \qquad \epsilon(\varsigma) = \sum_{k=2}^{\infty} \frac{\varsigma^k}{k.k!} \tag{10}$$

where $\gamma \approx 0.577216$ is the Euler-Mascheroni constant (removable from practical computations), ς may be an arbitrary real number and $x_1 = r\cos\phi$, $x_2 = r\sin\phi$, $x_3 = z$ with $r \geq 0$, $0 \leq \phi < 2\pi$ and arbitrary real z, neglecting the dependence of θ on ϕ and z and assuming (as a special case of (3)) constant initial temperature θ_0 everywhere. Let us consider Ω covering R^3 except the axis x_3. Inserting (9) into (7), we can see (MAPLE, MATLAB toolbox *symbolic* or similar software support can be recommended) that (7), degenerated to

$$\frac{\dot\theta}{\alpha} = \theta'' + \frac{\theta'}{r} \qquad \text{on } \Omega \times I\,, \tag{11}$$

is satisfied automatically; primes here mean $\partial/\partial r$. Nevertheless, (4) must be replaced by the physically motivated limit formulation

$$\lim_{r\to 0} \frac{-\lambda\theta'}{q_*(r)} = 1\,, \qquad q_*(r) = \frac{Q}{2\pi r}\,, \tag{12}$$

assuming the thermal power Q [W/m], related to the unit length on the axis x_3, occurring everywhere at the position $r = 0$, starting from $t = 0$.

These considerations can be generalized in several directions. Especially for an infinitely long cylinder Ω with the missing axis x_3 and with a finite diameter a (thus $0 < r < a < \infty$) [14] demonstrates how the standard Laplace transform is able to convert (11) to the analysis of certain Bessel equation; consequently we have to work with the Bessel functions of the first and second kind instead of exponential integrals (the limit passage $a \to \infty$ comes back to (9) naturally). However, all relevant quasi-analytical computational formulae are much more complicated than (9), thus their exploitation in inverse problems (as the aim of this paper) is rather limited.

3 An inverse problem

As a model inverse problem, let us consider a direct problem introduced in the previous section with these modifications: i) no values of λ and κ are known a priori (except some their rough initial

estimate), ii) in addition to (8) and (3) some values θ_* are prescribed on Γ, introduced as some surface (typically not included in $\partial\Omega$) in R^3. Considering some a priori weight functions $w \in L^\infty(\Gamma \times I)$ with values from [0,1] (related to preparation of real experiments), we can believe that the best available values of λ and κ correspond to the least-squares approach motivated minimum of

$$F(\lambda, \kappa) = \langle\langle \theta_{\lambda,\kappa} - \theta_*, w(\theta_{\lambda,\kappa} - \theta_*) \rangle\rangle \tag{13}$$

where $\langle\langle ., . \rangle\rangle$ refers to a scalar product in $L^2(\Gamma \times I)$ and $\theta_{\lambda,\kappa}$ is any solution of (8) and (3) for admissible λ and κ.

In particular, for constant values λ and κ we can introduce F in (13) as a (rather complicated) function of 2 real variables; in more general cases, namely those disturbing the linearity of (8), it must be considered as a functional defined on an appropriate infinite-dimensional function space. The pure linear case is studied in great details in [16] an in numerous references therein. For a priori given values of κ and sufficiently large Γ (with non-zero valuse of w) the dependence of λ on θ can be handled by [15] (although its approach has been suggested for capillary conduction, i. e. on the conservation of mass from the physical point of view, unlike the conservation of energy here).

Unfortunately, the quite general formulation (13) hides a lot of expectable difficulties: ill-possedness, numerical instability, need of artificial regularization, etc., as explained in [17], p. 255. Thus for practical identification of material characteristics the better choice is to pay attention to the careful organization of all experiments, to be able to make use of sufficiently simple computational formulae: in spherical coordinates for hot-ball measurements, in cylindrical coordinates for hot-wire measurements, like (9) here, in Cartesian coordinates for hot-plate measurements, etc. Another argument supporting this choice, important in this paper, is that an inexpensive experimental setting, covering all temperatures expectable in a thermal container, is not available, thus a series of measurements at several temperature levels, preserving nearly constant values of λ and κ, can represent a reasonable alternative.

Technical standards respect such arguments. By [8], coming from the above introduced cylindrical setting, we need:

a) a very long and thin heating wire of circular shape, whose thermal conductivity and capacity can be neglected,

b) a material specimen considerable as a very long rotational cylinder of large radius, whose axis lies just in the heating wire,

c) supplying to the specimen, starting from the zero time t, related to its unit length, to all directions, still the same thermal power Q, as needed by (9),

d) a material specimen prepared as homogeneous and isotropic for macroscopic calculations, with some effective values of scalar characteristics λ and α (and thus also κ),

e) all independent of θ in practice,

f) respecting (3) with constant θ_0.

Consequently (9) is applicable to corresponding direct calculations. For inverse ones, [8] works with the location of temperature sensor Γ degenerated to one point very close to the axis of rotation, i. e. lying just on the axis of the heating wire theoretically. This is impossible in practice, but needed only for the removal of all additive terms excepts the second one from the decomposition of $\mathrm{Ei}(.)$ in (10): if two temperatures by (9) in different times are subtracted, the first additive term vanishes and the third and all other terms are negligible, which gives

$$\theta(0,t)-\theta(0,t_\times)\approx\frac{Q}{4\pi\lambda}\ln\frac{t}{t_\times} \tag{14}$$

for any time $t\in I$ (except $t=0$ naturally) and some comparative time $t_*\in I$, different from t. Since the values $\theta_*(t)-\theta_*(t_\times)$ for r close to zero are available, at least for a large number of time steps $t\in I$ and one appropriate $t_\times\in I$, (14) is applicable to the evaluation of λ using the linear regression analysis, interpretable as a special case of minimization of F from (13) with missing κ; for the repeatability and certain improvements of such evaluations see [18].

The principal drawback of the identification procedure of λ based on (14) is the ignorance of the influence of κ or α. Moreover, the temperature is usually recorded also later when no thermal power is active, which is not exploited. As a potential remedy, following [14], let us consider Γ containing two sensors at some locations $r=r_1$ and $r=r_2$ where $0<r_1<r_2<\infty$; the temperature θ is recorded there for selected increasing positive values of time steps $t_1,\dots,t_m,\dots t_n$ where m and $n>m$ are some integer indices. We assume that the thermal power Q is active for $0<t\le t_m=\tau$, whereas the thermal power $-Q$ is active for $t\ge t_m$; thus the thermal power vanishes for $\tau<t\le T$. The aim now is to evaluate of λ and α thanks to the above announced temperature values $\theta_{*1k},\dots,\theta_{*mk},\dots\theta_{*nk}$.

During the hot-wire experiment Q is usually constant from $t=0$ up to $t=\tau$ where τ is some positive time. The temperature θ is recorded in some locations r_1 and r_2 for selected increasing positive values of time steps $t_1,\dots,t_m,\dots,t_n$ where m and $n>m$ are some integer indices: here we shall suppose that the thermal power Q is active for $0\le t\le t_m=\tau$, whereas the thermal power $-Q$ is active for $t\ge t_m$; consequently the thermal power vanishes for $t>\tau$.

The main aim is to identify unknown values of λ and α thanks to the above announced temperature values $\theta_{*1k},\dots,\theta_{*mk},\dots,\theta_{*nk}$ where the last index $k\in\{1,2\}$ refers to the 1st or 2nd sensor. The corresponding computed values in the same time steps are denoted by $\theta_{1k},\dots,\theta_{mk},\dots,\theta_{nk}$. Considering (for simplicity here) the time step t_m as the reference one, consequently for any $j\in\{1,\dots,m\}$ from (15) we obtain

$$\begin{aligned}\theta_j-\theta_m=&\frac{Q}{4\pi\lambda}\ln\frac{t_j}{t_m}+\frac{Q}{4\pi\lambda}\cdot\frac{1}{4\alpha r_k^2}\left(\frac{1}{t_j}-\frac{1}{t_m}\right)\\&-\frac{Q}{4\pi\lambda}\left(\epsilon\left(\frac{1}{4\alpha r_k^2t_j}\right)-\epsilon\left(\frac{1}{4\alpha r_k^2t_m}\right)\right).\end{aligned} \tag{15}$$

Repeating the same arguments to any $j\in\{m+1,\dots,n\}$, we receive similarly

$$\begin{aligned}\theta_j-\theta_m=&\frac{Q}{4\pi\lambda}\ln\frac{t_j}{t_j-t_m}+\frac{Q}{4\pi\lambda}\cdot\frac{1}{4\alpha r_k^2}\left(\frac{1}{t_j}-\frac{1}{t_j-t_m}\right)\\&-\frac{Q}{4\pi\lambda}\left(\epsilon\left(\frac{1}{4\alpha r_k^2t_j}\right)-\epsilon\left(\frac{1}{4\alpha r_k^2(t_j-t_m)}\right)\right).\end{aligned} \tag{16}$$

Clearly the formulae (15) and (16) are not suitable to direct evaluation of λ and α because of the lack of unicity and of and the need of some relaxation of the effect of random (or even system) measurement errors. Let us utilize the least squares approach, motivated by (13), again, with non-zero weights w_j on discrete time steps t_j where some indices j are taken from $1,\dots,m-1$ for (15) or from $m+1,\dots,n$ for (16); such indices are intended as admissible ones. Thus the two-step algorithm is available:

1) considering some reasonable estimates of λ and α in all right-hand side additive terms of (15) and (16) except the first ones, multiplying (15) by $w_j \ln(t_j/t_m)$ and (16) by $w_j \ln(t_j/(t_j - t_m))$ formally and summing up over all admissible j, from the result we are able to compute just one improved value of λ,
2) in the analogous way, knowing the estimates of λ and α in all right-hand side additive terms of (15) and (16) except the second ones, multiplying (15) by $w_j(1/t_j - 1/t_m)$ and (16) by $w_j(1/t_j - 1/(t_j - t_m))$ formally and summing up over all admissible j, from the result we are able to compute just one improved value of α.

In the usual configuration with r_1 close to zero (for certain compatibility with [8]) and $r_1 \ll r_2$, the following iteration algorithm is suitable: from some estimates α and λ to improve λ from the first sensor measurements, then to improve α from the second sensor measurements and to repeat such cycle until the differences between iterated values are not negligible.

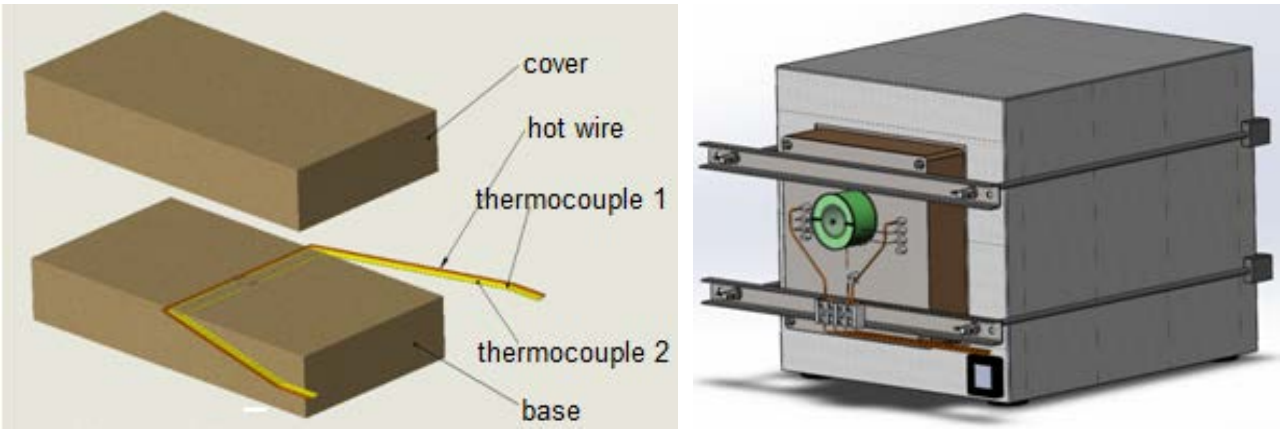

Fig. 2. Hot-wire experiment configuration (left scheme) and laboratory oven (right scheme).

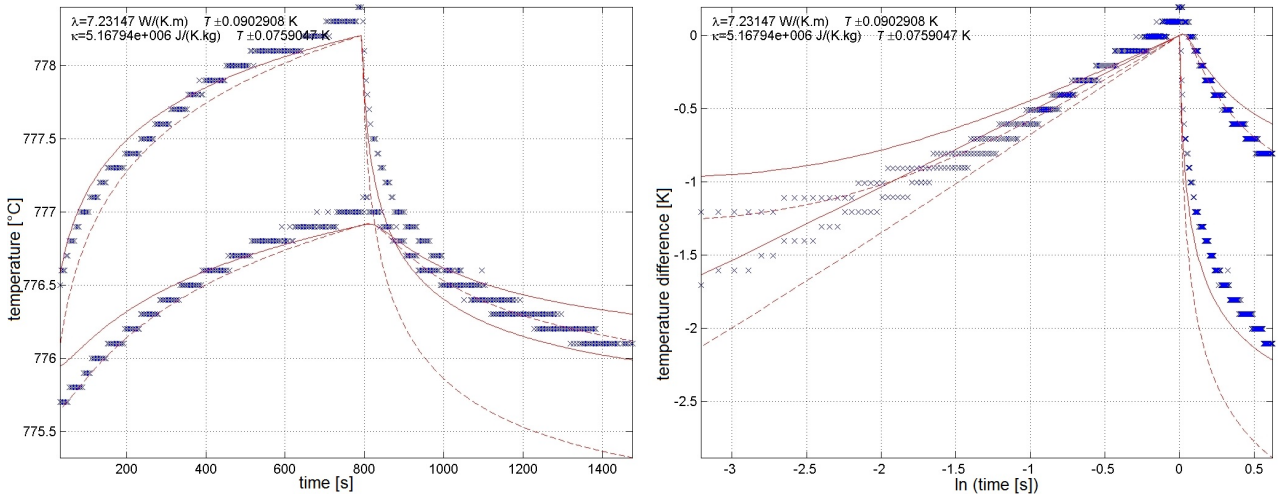

Fig. 3. Example of MATLAB-based identification procedure of λ and α for an experimental specimen at the reference temperature 786 °C: development of θ at 2 computational positions (left graph), also in the semilogarithmic scale (right graph).

4 Example of experimental and computational results

The practical configuration for high-temperature laboratory experiments is evident from Fig. 3; more technical details (including all oven components, their sizes, etc.) can be found in [7]. Unlike the heating kanthal (Fe, Cr, Al and Co alloy) wire, applied specimens have not (theoretically assumed) cylindrical shape, thus all experiments should work with T small enough, to suppress the effects of thermal transfer on their real exterior boundaries. The value of Q is not very substantial, but must be known a priori and stabilized carefully during every experiment.

The identification procedure for λ and κ (via α) has been written in MATLAB; no additional toolboxes are needed. Fig. 5 represents an illustrative example of its performance for one of a large number of tested specimens and temperature levels. The blue points correspond to the temperature records from both sensors with the sensibility 0.1 °C (thus they are seemingly piecewise constants). The dashed red curves correspond to the first rough estimate by (14); the linearity of the lower dashed curve in the semilogaritmic scale follows from (14) directly; all temperature differences are non-positive because of the reference temperature taken in the time τ (end of heating). The full red curves show the results obtained from the iteration procedure coming from (15) and (16).

Repeating such calculations several for a set of reference interior oven temperatures, here for (approximately) {20, 100, 200, 300, 400, 500, 600, 700, 800} °C, we are able to obtain the temperature dependence of λ and κ for (8), consequently to evaluate its preference for the utilization in a real thermal container. Fig. 5 corresponds to the material chosen by [7] finally: both dependences of λ and κ on θ are nearly linear for temperature values between 300 and 800 °C. Higher temperatures than 800 °C cannot be recommended because of the real danger of unwanted structural changes both in the tested specimens and in particular components of experimental equipment, especially due to the applied heating wire.

5 More general optimization tools

Practical minimization of F by (13), with the aim of identification of λ and κ, including their dependence on θ, relies on substantial physical and geometrical simplification here and the consequent availability of some explicit computational formulae, based on (9), unlike the application of general (e. g. finite element) numerical techniques on (8) with (3). However, in the design of thermal containers, even in the choice of materials for their performance, this can be seen as a very particular optimization result only. Thus the development of a more general optimization tool, as robust, effective and inexpensive as possible, cannot be avoided. Most technical solutions declared as optimized (including [7], referenced in the previous section), apply a simple selection from a finite (rather low) number of variants only, in particular in such cases when both non-trivial experiments and computations are needed to receive separate values of rather complicated goal functions, generalizing F from (13). incorporating various additional conditions thanks to penalty terms.

Some authors avoid the analysis of differential or integral equations at all, referring to some soft-computing approaches, as genetic algorithms, neural networks, etc.; for much more information and references corresponding to various problems of thermal transfer see [19] and [20]. Most modern optimization algorithms usual some exact or approximate evaluations of gradients, needing many evaluations of F (quasi-Newton iterations, conjugate gradient techniques, etc.), as analyzed in [21] in all details. A promising (although not very quick) algorithm in such situation seems to be the nonlinear simplex Nelder-Mead one, suggested in [22] originally, modified by [23] slightly, with 5 gradient-free steps: i) reflection, ii) expansion, iii) outside contraction, iv) inside contraction, all with just one additional evaluation of F, and (as the last choice) v) shrink, with p additional evaluations of

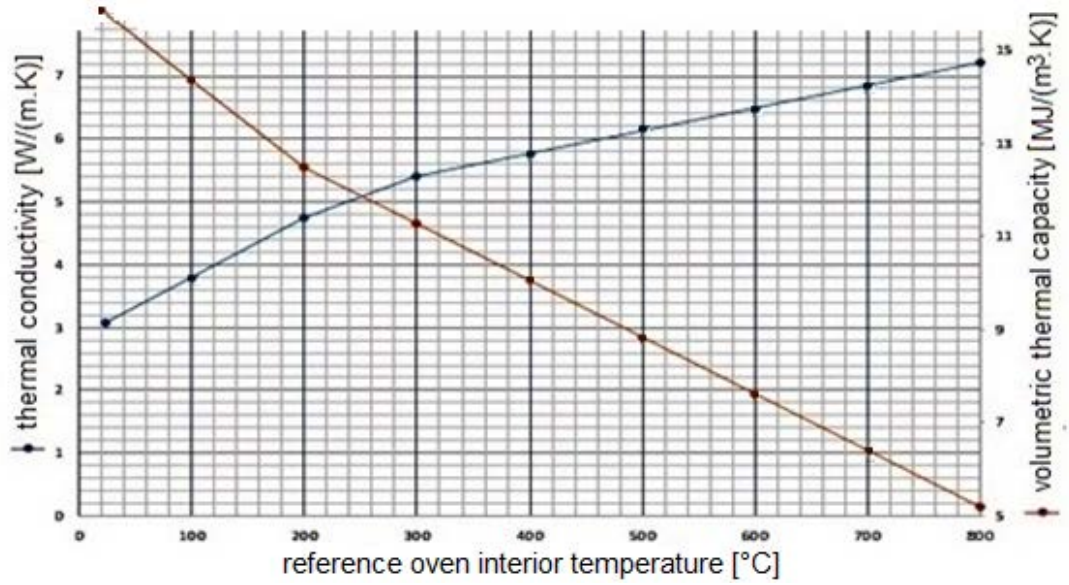

Fig. 4. Temperature dependence of λ and κ for the specimen with the following chemical composition: dominating 96.0 % MgO, further 2.2 % CaO, 0.5 % SiO_2, 0.5 % Fe_2O_3, 0.2 % Al_2O_3, etc. (0.6 % total); by the material data sheet of Slovmag a. s. Lubeník (Slovak Republic).

F where p refers to a number of optimized parameters. Unfortunately, the complete formal convergence proof of this algorithm is contained in [23] only for $p = 1$ (where every direction can be seen as a gradient one); the computer-supported 25-page proof for $p = 2$ in [24] does not allow any step ii) and cannot be extended to $p \in \{3, 4, \ldots\}$ in an intuitive way. Some artificial examples of stagnation or incorrect finishing of the algorithm can be overcome using certain adaptive parameters for steps i)–v), various conditional restarting, simplex regularization or reshaping strategies; most computations based on the MATLAB function *fminsearch* from the toolbox *optimization* and on similar software tools do not produce (at least evidently) wrong results. Consequently a frame-based method of [25] can be interpreted as a (rather complicated) always convergent variant of the Nelder-Mead algorithm. Moreover, the recent development (with still open questions) tries to combine some advantages of gradient and simplex algorithms, as sketched in [26].

Up to now, some partial results referenced in this section have been implemented to the design of controlled heating for passive, low-energy and similar buildings, depending on a rather low number p of optimized parameters, as documented by [27]. Their effective application to thermal containers needs deeper connection to advanced planning of numerous experiments and is still in development.

6 Conclusion

The paper documents the significance of development of the wide range of optimization methods, motivated by new development in civil engineering, compatible with increasing user comfort and sustainable development. The introduction to direct and inverse problems is accompanied by an instructive example of identification of material characteristics for thermal containers, as a part of research priorities at FCE BUT. However, partial results generate still other problems, stimulating the relevant research in the near future.

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