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INVERSE PROBLEMS OF HEAT TRANSFER*

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1 Introduction

Well-posed problems of heat transfer, much-favoured by most mathematicians, as an important class of simplified mathematical formulations of real physical processes, based on the conservation principles of classical mechanics, exploited in mechanical, electrical, civil etc. engineering, require the complete setting of i) initial conditions, ii) boundary conditions (prescribed temperature or heat flux everywhere) and iii) material characteristics. However, in engineering applications some data of types i), ii) or iii) are uncertain, inaccurate or missing. The remedy, coming from their reconstruction from some additional information, obtained from temperature or heat flux measurements, generate various classes of ill-posed problems with specific difficulties: even the apparently simple one-dimensional linearized model of heat propagation in a rod [6] needs non-trivial a priori estimates (valid under some additional regularity assumptions), combined truncation and regularization methods, to be able to apply the Schauder fixed point theorem.

The theoretical, experimental and computational analysis of inverse problems of heat transfer and related physical processes of the last decades has its own history: from different points of view it is monitored in [1], [3], [4] and [9]. In this paper we shall pay special attention to the missing data iii) in the analysis of insulation and accumulation properties of building materials (typically with a microscopically porous irregular structure), i.e. to the reliable identification of their basic macroscopic material characteristics. Following the Czech and European technical standards, we shall work with the thermal conductivity λ, heat capacity c and material density ρ, constant at least within certain reasonable temperature range, in an isotropic medium. Whereas the experimental setting of ρ is easy, the stationary measurements of λ and c do not give, according to the required measurement time, good results. The conventional non-stationary measurement equipments are expensive, use strange sets of calibration materials and their applicability to non-classical materials is limited. The development of alternative non-stationary identification methods (the frequency-domain method, the step-heating method, the hot-strip / hot-wire method, the infrared photography access, etc.) is documented in [1]. A class of primary inexpensive measurement devices, introduced in this paper, combines the hot-wire approach with the MATLAB-based numerical and computational support.

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2 Physical and mathematical preliminaries

Let us consider the 3-dimensional Euclidean space, supplied by the Cartesian coordinate system $x = (x_1, x_2, x_3)$, and a domain Ω in this space, occupied by a (macroscopically) homogeneous and isotropic material with unknown characteristics $a = \lambda/(c\rho)$ and $b = 1/\lambda$, whose (sufficiently smooth) boundary $\partial\Omega$ involves some parts Γ_D with prescribed boundary conditions of Dirichlet type

$$T(x,t) = T_*(x) \qquad \forall\, t \in I \;\; \forall\, x \in \Gamma_D \tag{1}$$

and Γ_N with those of Neumann type

$$\nabla T(x,t) \cdot \nu(x) + bq(t) = 0 \qquad \forall\, t \in I \;\; \forall\, x \in \Gamma_N \tag{2}$$

where $\nu(x)$ refers to a local unit outside normal vector.

Since any real measurement device consists of a finite number n of further material layers Ω_i with $i \in \{1, \ldots, n\}$ (cf. *Illustrative example*), the analogous notation can be applied to each i-th materials with prescribed characteristics a_i and b_i. Moreover, (2) holds also with the heat flux $q(t)$, occurring on some part $\Gamma \subseteq \partial\Omega \setminus \Gamma_N$ of the union of interfaces $\Omega \cap \Omega_1, \ldots, \Omega \cap \Omega_n$. Similar heat fluxes are present on mutual interfaces of $\Omega_1, \ldots, \Omega_n$. All such fluxes are not known explicitly, being determined from contact conditions; here we shall consider only perfect contacts with continuous temperature distributions.

Following Chap. 3 of [2], the principle of conservation of energy together with the empirical constitutive Fourier law gives

$$\dot{T}(x,t) - a\nabla^2 T(x,t) = 0 \tag{3}$$

where the dot symbol is reserved for a derivative with respect to t and $\nabla^2(\cdot)$ means $\mathrm{div}(\mathrm{grad}(\cdot))$ briefly; for $t = 0$ we shall consider $T(x,0) = T_e$ with the constant environmental temperature T_e and the same, i.e. $T(\cdot,t) = T_e$, should be true in any time $t \in I$ on all outer surfaces of the layered measurement device to guarantee a physically closed measurement system.

It is natural to search for $T(x,t)$ in the space of abstract functions $L^2(I,V)$, mapping I into some appropriate subspace V of the Sobolev space $W^{1,2}(\Omega)$, although better regularity results can be obtained – see [4, p. 256]. In the direct formulation with given material characteristics a and b the solvability of (3) with boundary conditions (1) and (2) and convergence properties of sequences of approximate solutions in finite-dimensional spaces follow, at least for the most frequently discussed case $\partial\Omega = \Gamma_D \cup \Gamma_N$ with $\Gamma_D \cap \Gamma_N = \emptyset$, from the Lax–Milgram theorem. Unfortunately, the inverse formulations with unknown a and/or b, or, alternatively, with partially unknown initial or boundary conditions, result typically in ill-conditioned mathematical problems and unstable numerical algorithms, as discussed in [4, p. 21].

For simplicity, let us assume that just both a and b are unknown, consequently infinitely many solution of (3) with boundary conditions (1) and (2) may exist.

Let us introduce the following notations of scalar products: $(\cdot,\cdot)$ in $L^2(\Omega)$ and in $[L^2(\Omega)]^3$, $\langle\cdot,\cdot\rangle$ in $L^2(\partial\Omega)$, $\langle\cdot,\cdot\rangle_D$ in $L^2(\Gamma_D)$, $\langle\cdot,\cdot\rangle_N$ in $L^2(\Gamma_N)$, $\langle\cdot,\cdot\rangle_I$ in $L^2(I,L^2(\Gamma))$. Applying any test function Φ (usually) from V to (3), the Green–Ostrogradskii theorem (at least in sense of distributions) gives $a^{-1}(\Phi,\dot{T})-(\Phi,\nabla^2 T)=0$, $a^{-1}(\Phi,\dot{T})+(\nabla\Phi,\nabla T)-\langle\Phi,\nabla T\cdot\nu\rangle=0$ and $a^{-1}(\Phi,\dot{T})-(\nabla^2\Phi,T)-\langle\Phi,\nabla T\cdot\nu\rangle+\langle\nabla\Phi\cdot\nu,T\rangle=0$; thus by (1) and (2) we have

$$a^{-1}(\Phi,\dot{T})-B(\Phi,T)=b\langle\Phi,q\rangle_N-\langle\nabla\Phi\cdot\nu,T_*\rangle_D\,. \tag{4}$$

for $B(\Phi,T):=(\nabla^2\Phi,T)+\langle\Phi,\nabla T\cdot\nu\rangle_D-\langle\nabla\Phi\cdot\nu,T\rangle_N$.

The ideal final aim is to find $T\in L^2(I,V)$, together with real constants a and b, satisfying (4) and (2). More realistic approaches try to satisfy (2) (or rarely (4)) in some weaker (inaccurate) sense – for the detailed overview see [1]. We shall apply the least squares technique, minimizing

$$F(a,b)=\frac{1}{2}\langle bq+\nabla T(a,b)\cdot\nu,bq+\nabla T(a,b)\cdot\nu\rangle_I\,; \tag{5}$$

F here is only a real function of two variables a and b, $T(x,t)$ from (4) depend on parameters a and b, thus we have $T(x,t,a,b)$ now, omitting the first two variables x and t for brevity; the rectangular quadrature rule on I in $m+1$ nodes $t=jh$ for $j\in\{0,1,\ldots,m\}$ and $h:=\tau/m$ is needed in practice. The first and second derivatives of F,with respect to a and b, i.e. $F_{,a}(a,b)$, $F_{,b}(a,b)$, $F_{,aa}(a,b)$, $F_{,ab}(a,b)$ and $F_{,bb}(a,b)$, can be then evaluated from the first and second temperature derivatives $T_{,a}(a,b)$, $T_{,b}(a,b)$, $T_{,aa}(a,b)$, $T_{,ab}(a,b)$ and $T_{,bb}(a,b)$. In the case of lack of boundary data (when F becomes a more general functional), some (rather complicated) iterative procedures are available, e.g. that based on the conjugate gradient algorithm applied to direct, adjoint and sensitivity problems in [9, p. 21].

3 Computational algorithm

If some reasonable estimate of the characteristics a and b is available, we can apply the Newton algorithm to obtain their improved values $a^\star$ and $b^\star$ in the well-known form

$$\begin{bmatrix} F_{,aa}(a,b) & F_{,ab}(a,b)\\ F_{,ab}(a,b) & F_{,bb}(a,b)\end{bmatrix}\cdot\begin{bmatrix} a^\star-a\\ b^\star-b\end{bmatrix}=-\begin{bmatrix} F_{,a}(a,b)\\ F_{,b}(a,b)\end{bmatrix}. \tag{6}$$

The derivatives included in this formula should be as simple as possible.

Namely if $\partial\Omega=\Gamma_D=\Gamma$ and $\Gamma_N=\emptyset$ then T is independent of b and all derivatives of F vanish or simplify substantially. For the discretization on Ω the finite element technique using the Hermite polynomials and the set of discrete unknown variables $\psi:=(T,\nabla T)$ is available. Applying the Crank–Nicholson scheme, for any $j\in\{1,\ldots,m\}$ we obtain

$$\frac{1}{ah}N(\psi_j-\psi_{j-1})-\frac{1}{2}K(\psi_j+\psi_{j-1})=\frac{1}{2}(g_j+g_{j-1}) \tag{7}$$

with certain real symmetric sparse square matrices N and K and corresponding real vectors $g_0, g_1, \dots g_m$ (dependding on the choice of finite element mesh on Ω), i.e. briefly $S\psi_j = Q\psi_{j-1} + \gamma_j$ with $M := N/h$, $S := a^{-1}M - K/2$, $Q := a^{-1}M + K/2$ and $\gamma_j := (g_j + g_{j-1})/2$. Consequently we receive $S\psi_{j,a} = Q\psi_{j-1,a} + a^{-2}M(\psi_j - \psi_{j-1})$ and $S\psi_{j,aa} = Q\psi_{j-1,aa} + 2a^{-2}M(\psi_{j,a} - \psi_{j-1,a}) - 2a^{-3}M(\psi_j - \psi_{j-1})$. Thus (7) enables us to evaluate all a-derivatives of T and ∇T required in (6).

The 2- and 3-dimensional configurations typically do not admit $\Gamma_N = \emptyset$. Moreover, the heat fluxes $q(t)$ in the modified (2) are available (unlike those from the original (2)) only indirectly, from solutions of (4) on Ω_i with $i \in \{1, \dots, n\}$ instead of Ω; this will be highlighted using the index i. Let us assume $\Gamma = \Gamma_D$ and $\Gamma_N = \Gamma \setminus \Gamma_D \neq \emptyset$. Then (4) gets the form $a^{-1}(\Phi, \dot{T}) - B(\Phi, T) = b\langle \Phi, q\rangle_N - \langle \nabla\Phi \cdot \nu, T_*\rangle_D$, $a_i^{-1}(\Phi, \dot{T})_i - B(\Phi, T)_i = b_i\langle \Phi, q\rangle_{Ni} - \langle \nabla\Phi \cdot \nu, T_*\rangle_{Di}$ for all $i \in \{1, \dots, n\}$. Thanks to the identity of heat fluxes on all nonempty sets $\partial\Omega \cup \partial\Omega_i$ and $\partial\Omega_i \cup \partial\Omega_k$ with $i, k \in \{1, \dots, n\}$ all remaining $q(t)$ can be eliminated to receive $\psi_1, \dots, \psi_n$ from the analogy of (7) as functions of a and linear functions of b (not only functions of a as in the preceding case); for the detailed structure of corresponding linear systems (involving both thermal conduction and convection) see [3, p. 116]. This approach enables us to define S, Q, γ_j, etc., in the same way as from (7) again; their linear dependence on b guarantees that the formulae for the evaluation of derivatives of F (using the numerical quadrature on $\Gamma_D \times I$) with respect to a and b do not disturb the efficiency of the algorithm (6).

The same algorithm offers the possibility of quick evaluation of changes of a and b forced by the modified input data. The variance-based sensitivity analysis (the construction of Sobol indices) by [5] can be then useful to study the effect of stochastic uncertainty on the resulting a and b. However, the general approach considers the variables $q(x, t, \theta)$, $T(x, t, \theta)$, etc. also as functions of parameters θ from the sample space Θ of elementary events; such sample space must be supplied by the minimal σ-algebra on Θ and by certain probability measure P. Then it is possible to replace $F(a, b)$ from (5) by

$$F(a, b) = \frac{1}{2}\int_\Theta \langle bq + \nabla T(a, b) \cdot \nu, bq + \nabla T(a, b) \cdot \nu\rangle_I \, \mathrm{d}P \tag{8}$$

and apply some uncertainty representation technique to (8), as the Karhunen-Loève or polynomial chaos expansions by [9, p. 10], or, alternatively, a Bayesian approach by [9, p. 25].

4 Illustrative example

The basic configuration of the measurement device, suggested originally in [8], consists of the following layers: 1. thick insulation layer (polystyrene), 2. active heating plate (aluminium), 3. material specimen (with unknown material characteristics), 4. passive additional plate (aluminium), 5. thick insulation layer (polystyrene). The interfaces 1./2. and 4./5. contain two sets of temperature sensors recording the

temperature $T_*(t)$ at (in practice discrete) times t from the time interval $I = [0, \tau]$ of a given length τ. The interface 1./2. hides also a carefully controlled built-in generator of time-variable heat flux $q(t)$ for the same times t. However, such configuration is not acceptable e.g. for the measurements of maturing silicate mixtures in massive structures in situ: the remedy is to remove 4. and 5., considering the real massive structure (nearly the half-space) instead of 3.

The above sketched special geometrical configuration is typical just for such one-dimensional simplified systems with parallel layers, here especially $n = 4$. Unlike the formally complicated algorithm of [7], coming from the a priori known temperatures on the boundary of 1. and 5. and from the temperatures and heat fluxes at the left side of 2. and right side of 4., we are able to prescribe the temperature at the whole boundary of 3.

Fig. 1 and Fig. 2 show the results of identification of a and b from the experiment, lasting $\tau = 300\,\mathrm{s}$. The first half of both Fig. 1 and Fig. 2 refers to the new building material specimen, tested at the Faculty of Civil Engineering of Brno University of Technology (resulting $a = 1.09377 \cdot 10^{-6}\,\mathrm{m^2/s}$, $b = 2.05909 \cdot 10^{1}\,\mathrm{m{\cdot}K/W}$), the second one to the mineral wool, whose properties are similar to polystyrene (resulting $a = 6.55382 \cdot 10^{-7}\,\mathrm{m^2/s}$, $b = 1.13620\,\mathrm{m{\cdot}K/W}$), as the test of algorithm robustness only: the strongly insulated heating device from both sides causes the low accuracy of recorded temperature differences. The experimental heating was very special: constant for $t \in [0, 300]\,\mathrm{s}$, zero for $t \in [300, 600]\,\mathrm{s}$. Fig. 1 shows the redistribution of temperature, its gradient and heat flux in the whole measurement system in time: full lines for $t \in [0, 300]\,\mathrm{s}$, dotted lines otherwise. Fig. 2 demonstrates the least-squares-based fitting of computed interface values of heat flux with corresponding experimental data. The complete original software code has been written in MATLAB (without any additional packages).

5 Conclusions

The paper presents the mathematical preliminaries and the computational support for a rather general class of heat transfer problems, especially in building materials. An illustrative example demonstrates the MATLAB-based support for the identification of material characteristics, i.e. for the missing information iii) from *Introduction*. This approach is open to further generalization: to the analysis of anisotropic material (λ becomes a real square symmetrical matrix), interface heat convection (new material characteristics of interfaces occur), temperature-dependent material characteristics, etc.

The proper mathematical analysis, including both the existence of solutions and the convergence of sequences of approximate solutions in finite-dimensional function spaces, constructed from the algorithm of above sketched type, contains still open questions. However, the aim of sufficient generalization of the results of type [6] seems to be realistic. The relevant analysis in probabilistic measures (instead of standard Lebesgue ones) is needed, too, to handle the evaluation of uncertainty of identified characteristics.

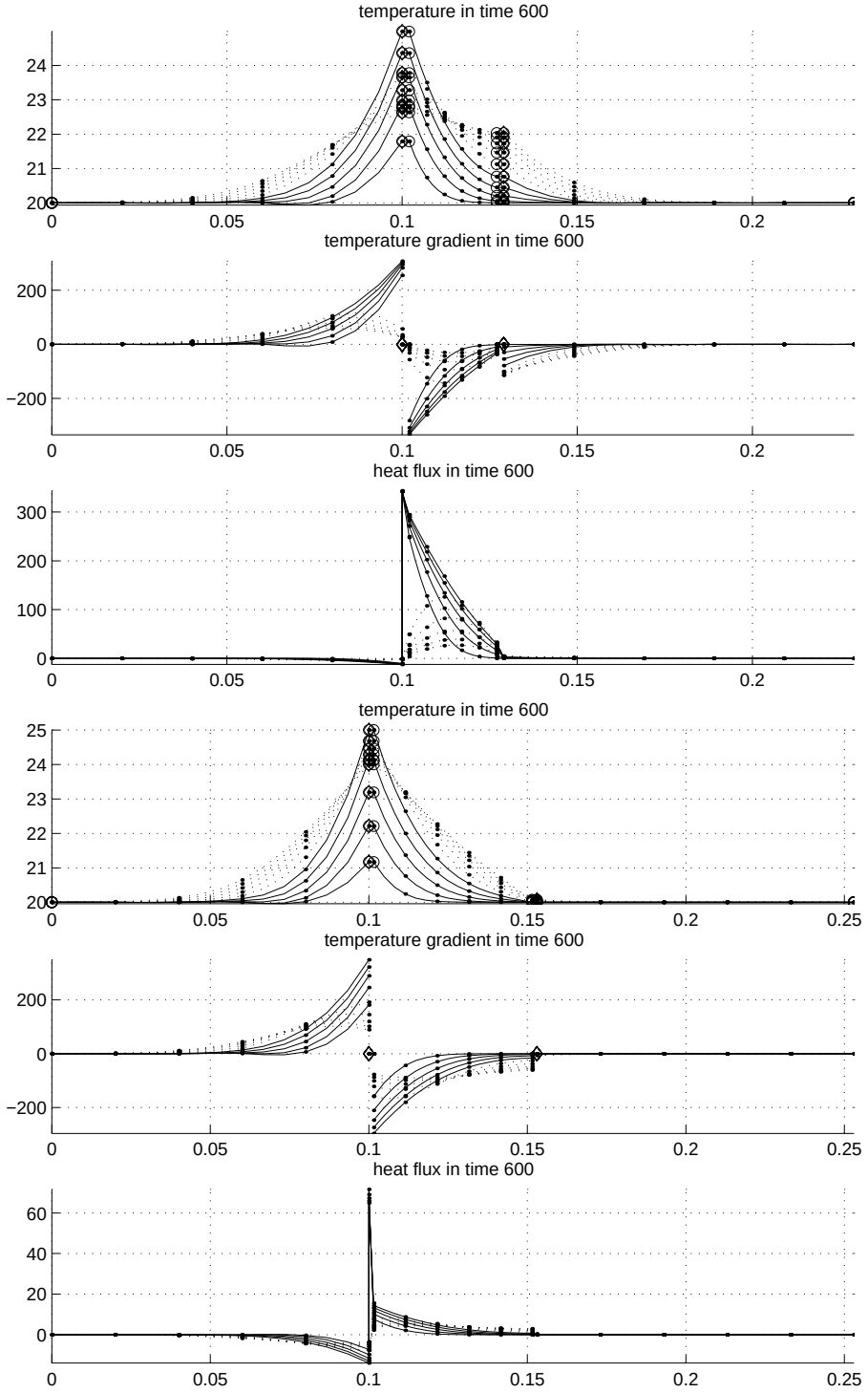

Fig. 1: *Temperature, its gradient and heat flux x-redistribution in time.*

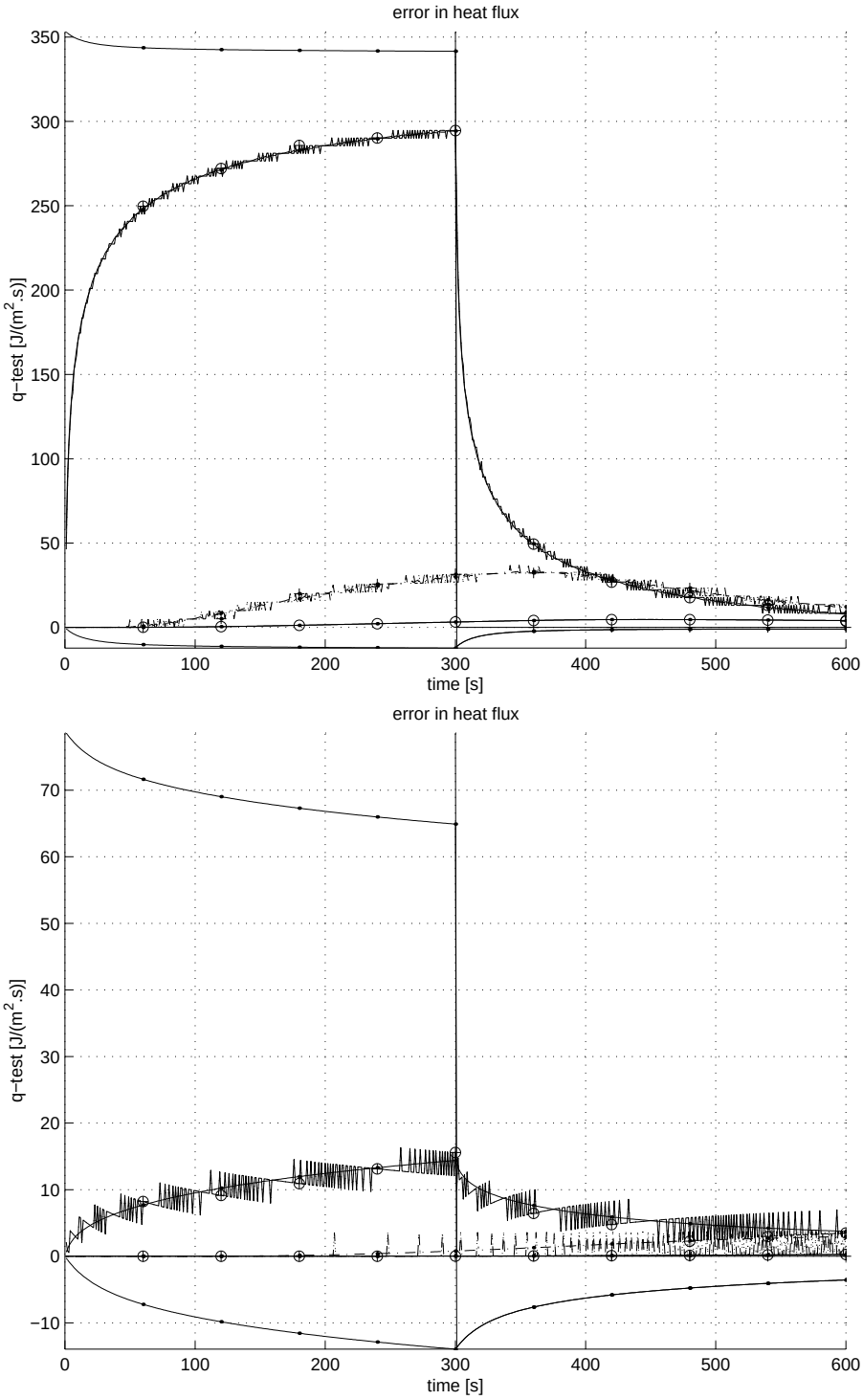

Fig. 2: *Fitting of computed interface values of heat flux with experimental data.*

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