Simultaneous reconstruction of space-dependent heat transfer coefficients and initial temperature

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Abstract

Many complex physical phenomena and engineering systems, e.g., in heat exchanges, reflux condensers, combustion chambers, nuclear vessels, etc., due to the high temperatures/high pressures hostile environment involved, possess certain properties which are inaccessible to measure and therefore their influence/determination using inverse analysis is very important and desirable. In this spirit, the purpose of this paper is to mathematically formulate and analyse a new inverse problem in which given measurements of temperature at two different instants, it is required to obtain the space-dependent heat transfer coefficients (HTCs) and the initial temperature. This simultaneous identification is challenging since it is both nonlinear and ill-posed. The uniqueness of solution is established based on the max-min principle for parabolic equations and the contraction mapping principle for the existence and uniqueness of a fixed point. The novel inverse mathematical model that is proposed offers appropriate scientific guidance to the polymer/heat transfer processing industry as to which data to measure/provide in order to be able to reliably determine the desirable HTCs along with the initial temperature, which is in general unknown. Furthermore, for the reconstruction, the surface HTC is determined separately, whilst the variational formulation is introduced for the simultaneous determination of the domain HTC and the initial temperature. The Fréchet gradient of the minimising objective functional is derived. The numerical reconstruction process is based on the conjugate gradient method (CGM) regularized by the discrepancy principle. Accurate and stable numerical solutions are obtained even in the presence of noise in the input temperature data. Since noisy data are invented, the study models realistic practical situations in which temperature measurements recorded using sensors or thermocouples are inherently contaminated with random noise.

Keywords: Inverse problem; Heat transfer; Conjugate gradient method; Heat transfer coefficients; Initial temperature

1. Introduction

Managing and controlling the complex process of heat transfer involves solving a wide-range of inverse problems concerned with the identification of physical properties and heat transfer coefficients, internal sources, boundary and/or initial conditions [1]. In particular, the efficient and safe performance of heat transfer apparatus and equipment requires knowledge of the HTCs.

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Therefore, an important but difficult problem of reconstructing the domain and surface HTCs [2], which are assumed to be spacewise dependent, from temperature measurements at interior points inside the heat conductor at prescribed times is proposed. This approach is practically advantageous because only internal temperature data at a couple of distinct times are required to be measured, while the exterior information about the fluid flow is not necessary [3]. Furthermore, despite recent advances, modern technology such as forging (including quenching) that is currently employed for heat treatment of aircraft or car parts, can cause cracks in the material due to the rapid cooling high-pressure gas quenching [4]. In such a current situation of heat treatments mainly based on practical engineering experience and technical know-how, the development of inverse expert techniques/models capable to predict the quality of the treated parts is very timely and important, as it would result in increased productivity (savings in time, cost and energy), as well as in planning new and better conditions for future treatments. On the other hand, the price to pay is that a challenging mathematical problem has to be solved, with the difficulty lying not only in the fact that the noisy data that is measured has to be carefully analysed both quantitatively and qualitatively in order to guarantee uniqueness and stability of the solution, but also due to the fact that inverse parabolic heat transfer problem is nonlinear in addition to being ill-posed. Moreover, in certain applications, e.g., steel melting, data assimilation or deblurring, the initial status of the diffusion process cannot be prescribed directly, but instead the temperature at a later time is available. This latter backward heat conduction problem (BHCP) is also well-known to be severely ill-posed, [5]. The inverse modelling performed in this study will impact the inverse problems community concerned with engineering applications of optimal heat transfer design inside building enclosures [6], quenching heat treatment [7], thermal spacecraft protection and safeness of nuclear reactors, [8], and improving the efficiency of heat exchanger fins [9] or heat flux gauges in wind-tunnel facilities [10].

When the initial temperature is known, the inverse problem concerning the identification of the potential/radiative/blood perfusion coefficient from final temperature measurements was theoretically investigated in [11, 12, 13, 14], where the uniqueness of solution under various sufficient conditions and various spaces of functions were established. Moreover, in [15, 16] generic local well-posedness of the inverse problem was established. Under the particular case that the coefficient additively separates a conditional Lipschitz stability of its recovery was established in [17]. In [18], the unknown coefficient was numerically reconstructed by minimizing the nonlinear Tikhonov regularization functional. In [19], the same inverse problem as in [18] was considered from discrete final temperature observations. On the basis of an interpolation technique, a new method was found to reconstruct the coefficient by minimizing the same Tikhonov regularization functional. In [20], the radiative coefficient was determined by minimizing a different weighted objective gradient functional. The coefficient was obtained numerically by applying the Armijo algorithm combined with the finite element method (FEM). Recently, this coefficient was numerically determined from final or time-average temperature measurements using the conjugate gradient method (CGM) in [21].

On the other hand, when all coefficients in the governing parabolic PDE are known, but the initial temperature is unknown and has to be determined from final temperature data, the resulting BHCP is well-known to be severely ill-posed. However, conditions under which it can become stable are well-known [5, 22]. Moreover, there are many numerical techniques for reconstructing the unknown initial temperature, which include the iterative CGM [23, 24], the boundary element method (BEM) [25], the elliptic approximation together with the BEM [26], the Tikhonov regularization approach [27], the Fourier regularization method [28], and the non-local boundary value problem method [29]. It is also worth noting [30] for the solution of the BHCP for the heat equa-

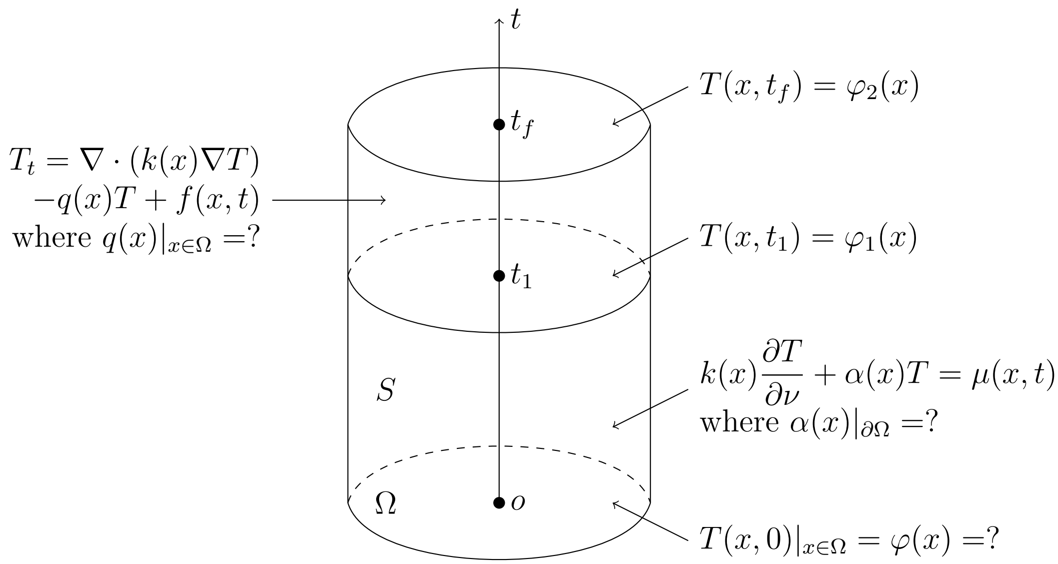

Figure 1: Schematic of the inverse problem under investigation.

tion with heterogeneous thermal conductivity and the more recent investigation [31] of the BHCP for the nonlinear heat equation. The inversion of statistical discrete final temperature measured data to obtain the initial temperature has also been considered recently in [32].

Prior to this study, the space-dependent heat (thermal) radiative coefficient, which in this paper is renamed as the domain HTC, and the initial temperature were simultaneously reconstructed in [33] from temperature measurements at a fixed time and in a subregion of the space-time domain. The stability of the inverse problem and the existence of a minimizer to the Tikhonov's first-order regularization functional were proved. The multi-grid gradient method was used to obtain the numerical solution of the nonlinear finite element minimization problem. In a subsequent paper [34], the previous domain HTC and the initial temperature were determined simultaneously with the surface HTC, which appears in a convection Robin boundary condition, from final time measurements only, provided that the domain HTC is *a priori* known on a sub-domain of the heat conductor. The uniqueness and stability for this inverse problem were obtained.

Compared to previous studies, in our investigation, we employ less information than in [33, 34], given by temperature observations at the final time t_f and at a instant of time t_1, where $t_1 \in (0, t_f)$. This is a completely new inverse problem, sketched in Figure 1, which has never been investigated before, so the first novelty of our study consists in the mathematical formulation. The uniqueness of the surface HTC in this inverse problem is obtained from the compatibility conditions, while noticing that other types of boundary measurements of the temperature or average temperature have been considered elsewhere [35, 36, 37]. Another novelty consists in proving that the domain HTC is unique. The is accomplished from the contraction mapping principle for the problem in the time-layer $[t_1, t_f]$. Finally the initial temperature is obtained uniquely from the energy estimate for the BHCP in the time-layer $[0, t_1]$. Next, the simultaneous numerical reconstruction of the domain HTC and the initial temperature represents another novelty of the paper. This is carried out by minimizing the Tikhonov-type objective functional with the already determined surface HTC. The final novelties of the paper consist in obtaining the Fréchet gradient components with respect to the two unknowns based on the solution of the adjoint problem, and the numerical implementation of the CGM. Since the inverse problem is nonlinear and unstable, the CGM is regularized by the discrepancy principle [23, 24] to obtain a stable and accurate numerical solution.

The plan of the paper is as follows. The mathematical formulation of the multi-component inverse problem under investigation is presented in section 2 together with the uniqueness result for the inverse problem. The variational formulation and the iterative CGM based on the sensitivity and adjoint problems and the gradient of the objective functional are presented in Sections 3 and 4. Numerical results are presented and discussed in Section 5 and finally, Section 6 highlights the conclusions of the work.

1.1. Notations and preliminaries

For $\Omega \subset \mathbb{R}^N, N = 1, 2, 3$, bounded domain with smooth boundary $\partial\Omega$, denote by $C^l(\Omega)$ for $l \in (0, 1)$, the Hölder space [38, 39] of all continuous functions $g(x)$ on Ω with Hölder exponent l, equipped with the norm

$$\|g\|_{C^l(\Omega)} := \sup_{x\in\Omega} |g(x)| + \sup_{x,x'\in\Omega, x\neq x'} \frac{|g(x) - g(x')|}{|x - x'|^l}.$$

For $m \in \mathbb{N}$, denote by $C^{m+l}(\Omega)$ the class of functions g satisfying $\partial_x^j g \in C^l(\Omega)$ for $0 \le |j| \le m$ with the norm

$$\|g\|_{C^{m+l}(\Omega)} := \sum_{|j|\le m} \|\partial_x^j g\|_{C^l(\Omega)},$$

where ∂_x^j denotes any partial derivative of $g(x)$ with respect to x of order j.

Let $t_f > 0$, then for the cylinder $Q := \Omega \times (0, t_f)$, the Hölder space $C^{l,l/2}(Q)$ is the Banach space of all continuous functions $u(x, t)$ in Q with the finite norm

$$\|u\|_{C^{l,l/2}(Q)} := \sup_{(x,t)\in Q} |u(x, t)| + \sup_{(x,t),(x',t)\in Q, x\neq x'} \frac{|u(x, t) - u(x', t)|}{|x - x'|^l} + \sup_{(x,t),(x,t')\in Q, t\neq t'} \frac{|u(x, t) - u(x, t')|}{|t - t'|^{l/2}}.$$

We can also denote by $C^{m+l,(m+l)/2}(Q)$ the Banach space of functions $u(x, t)$ that are continuous in Q with $\partial_t^r \partial_x^j u \in C^{l,l/2}(Q)$ for $0 \le 2r + |j| \le m$, equipped with a norm

$$\|u\|_{C^{m+l,(m+l)/2}(Q)} = \sum_{2r+|j|\le m} \|\partial_t^r \partial_x^j u\|_{C^{l,l/2}(Q)}.$$

2. Mathematical formulation and analysis

In the bounded conductor $\Omega \subset \mathbb{R}^N$ with boundary $\partial\Omega \in C^{2+l}$, consider the transient heat transfer process given by the following mathematical model:

$$\begin{cases} \dfrac{\partial T}{\partial t}(x, t) - \nabla \cdot (k(x)\nabla T(x, t)) + q(x)T(x, t) = f(x, t), & (x, t) \in \Omega \times (0, t_f) := Q, \\ k(x)\dfrac{\partial T}{\partial \nu} + \alpha(x)T(x, t) = \mu(x, t), & (x, t) \in \partial\Omega \times [0, t_f] := S, \\ T(x, 0) = \varphi(x), & x \in \overline{\Omega}, \end{cases} \tag{2.1}$$

where ν is the outward unit normal to the boundary $\partial\Omega$, $0 < k_0 \le k(x) \in C^{1+l}(\overline{\Omega})$, with k_0 a given positive constant, represents the thermal conductivity, $0 \le q(x) \in C^l(\Omega)$ and $0 \le \alpha(x) \in C^{1+l}(\partial\Omega)$ represent the domain and surface HTCs, respectively, and $f(x, t)$, $\mu(x, t)$ and $\varphi(x)$ represent an internal source, heat flux and initial temperature, respectively. For simplicity, the heat capacity has been assumed constant and taken to be unity. The Robin convective boundary condition in (2.1) (assuming, for simplicity, that the ambient temperature is constant and taken to be zero) involving the surface HTC, $\alpha(x)$ on $x \in \partial\Omega$, is the most important boundary condition for quenching process simulation [6]. In principle, if thermal imaging is used to measure the time-history of both the temperature and the heat flux on a subportion of the boundary $\partial\Omega$, then the surface HTC could be obtained directly by solving a non-characteristic Cauchy problem of the heat equation, [40]. However, in our paper, we consider space-dependent measurements at fixed times instead of Cauchy data boundary measurements. We also mention that in the analysis of this paper, the physical quantities $k(x)|_{x\in\Omega}$, $q(x)|_{x\in\Omega}$ and $\alpha(x)|_{x\in\partial\Omega}$ are assumed spatially distributed, but they can also be time-, space- and time-, or temperature-dependent [41, 42, 43, 44, 45, 46, 47].

For known functions $(k(x), q(x), \alpha(x))$, if we consider (f, μ, φ) as the inputs for the heat conduction process, then (2.1) defines a well-posed process, namely, the temperature solution $T(x,t)$ to (2.1) is well-defined. However, in some engineering situations, the system parameters as well as some inputs may be unknown. To be precise, we assume that the thermal conductivity $k(x)$ is known, but $q(x)$ and $\alpha(x)$ together with $\varphi(x)$ are unknown and have to be determined from some additional information that needs to be supplied. We are interested in the determination of $(q(x), \alpha(x), \varphi(x), T(x,t))$ satisfying (2.1), given the extra temperature measurements at some internal prescribed time $t_1 \in (0, t_f)$ and at the final time $t = t_f$, namely,

$$T(x,t_1) = \varphi_1(x), \quad T(x,t_f) = \varphi_2(x), \quad x \in \overline{\Omega}. \tag{2.2}$$

A sketch of the inverse problem under investigation is presented in Figure 1. A wide range of methods and specific devices for practical temperature measurements, such as (2.2), are described in [48].

Remark 1. *A weighted time-average temperature observation $\phi_2(x) = \int_{t_1}^{t_f} \omega(t)T(x,t)dt$ for $x \in \overline{\Omega}$, with $\omega > 0$ a given weight function, may be specified in place of the second condition $T(x,t_f) = \varphi_2(x)$ for $x \in \overline{\Omega}$, in* (2.2)*, [14, 21]. Note that the input data* (2.2) *and the output components $q(x)$ and $\varphi(x)$ of the inverse problem are both spatially distributed for $x \in \Omega$ and therefore, the rule of thumb of trace functionals in prescribing the extra data with respect to the unknowns is followed [49]. In case the destructive temperature measurements* (2.2) *are not permitted or available, non-destructive boundary temperature (or heat flux) measurements can be used instead, but this resulting non-characteristic, nonlinear and ill-posed inverse problem is deferred to a future work (a starting point could be perhaps combining the separate identification of the domain HTC $q(x)$ [50] with that of recovering the initial temperature $\varphi(x)$ [51]).*

In practical cases, measurements unavoidably contain some noise. Therefore, from the numerical implementation point of view, we are in fact seeking the solution only approximately from the noisy data $(\varphi_1^\delta, \varphi_2^\delta)$ of (φ_1, φ_2) satisfying

$$\|\varphi_1^\delta - \varphi_1\|_{L^2(\Omega)} \le \delta, \quad \|\varphi_2^\delta - \varphi_2\|_{L^2(\Omega)} \le \delta, \tag{2.3}$$

where $\delta \ge 0$ represents the noise level.

In summary, our inverse problem is to identify the HTCs, $\alpha(x)|_{x\in\partial\Omega}$ and $q(x)|_{x\in\Omega}$, the initial status $\varphi(x)|_{x\in\Omega}$, and the temperature $T(x,t)|_{(x,t)\in Q}$, from (2.1), and (2.2) or the noisy data $(\varphi_1^\delta, \varphi_2^\delta)$ satisfying (2.3). To analyse the above inverse problem, we need the following well-posedness result for the direct problem (2.1) (see [38], p.320).

Lemma 1. *Suppose $0 < k_0 \le k \in C^{1+l}(\Omega)$, $0 \le q \in C^l(\Omega)$ and $0 \le \alpha \in C^{1+l}(\partial\Omega)$. Then, for given $f \in C^{l,l/2}(Q)$, $\varphi \in C^{2+l}(\Omega)$, $\mu \in C^{1+l,(1+l)/2}(S)$ satisfying the compatibility conditions of order $[(l+1)/2]$, the direct problem (2.1) has a unique solution $T \in C^{2+l,1+l/2}(Q)$, which satisfies the estimate*

$$\|T\|_{C^{2+l,1+l/2}(Q)} \le c\left(\|f\|_{C^{l,l/2}(Q)} + \|\varphi\|_{C^{2+l}(\Omega)} + \|\mu\|_{C^{1+l,(1+l)/2}(S)}\right). \tag{2.4}$$

Notice that the inverse problem (2.1) and (2.2) is nonlinear when the triplet (q, α, φ) is unknown. We first establish the uniqueness for this inverse problem. To this end, we define the admissible set for the unknowns where we have the uniqueness. Define

$$\mathcal{Q} := \{q(x) : q \in C^l(\Omega), 0 < q^- \le q(x) \le q^+\}, \quad \mathcal{A} := \{\alpha(x) : 0 \le \alpha \in C^{1+l}(\partial\Omega)\}$$

and

$$\Phi := \{\varphi(x) : 0 < \varphi_0 \le \varphi \in C^{2+l}(\Omega)\},$$

where $q^{\pm}$ and φ_0 are given positive constants. We have the following uniqueness result.

Theorem 1. *For known and given $0 < k_0 \le k \in C^{1+l}(\Omega)$, $0 < f_0 \le f \in C^{l,l/2}(Q)$ and $0 \le \mu \in C^{1+l,(1+l)/2}(S)$, the solution to the inverse problem (2.1) and (2.2) is unique in $\mathcal{Q}\times\mathcal{A}\times\Phi$. That is, for $(T^i(x,t_1) = \varphi_1^i(x), T^i(x,t_f) = \varphi_2^i(x))$ being the inversion input data corresponding to $(q^i, \alpha^i, \varphi^i) \in \mathcal{Q}\times\mathcal{A}\times\Phi$ for $i = 1, 2$, we have that $(q^1, \alpha^1, \varphi^1) = (q^2, \alpha^2, \varphi^2)$ in $C^l(\Omega) \times C^{1+l}(\partial\Omega) \times C^{2+l}(\Omega)$, if $(\varphi_1^1(x), \varphi_2^1(x)) = (\varphi_1^2(x), \varphi_2^2(x))$.*

Proof. By the max-min principle for parabolic equations, for $(q^i, \alpha^i, \varphi^i) \in \mathcal{Q}\times\mathcal{A}\times\Phi$ together with $f \ge f_0 > 0$, $k \ge k_0 > 0$ and $\mu \ge 0$, it yields that $T^i(x,t) \ge T_0 > 0$ for $(x,t) \in \overline{Q}$, where the constant $T_0 = T_0(\varphi_0, f_0, k, \mu)$.

Using the Robin boundary condition for $T^i(x,t)$ at the internal time $t_1 \in (0, t_f)$, we have

$$k(x)\left(\frac{\partial T^1(x,t_1)}{\partial\nu} - \frac{\partial T^2(x,t_1)}{\partial\nu}\right) + (\alpha^1(x) - \alpha^2(x))T^1(x,t_1) = \alpha_2(x)(T^2(x,t_1) - T^1(x,t_1)), \quad x \in \partial\Omega.$$

However, by Lemma 1 we have that $\varphi_1^i(x) = T^i(x,t_1) \in C^{2+l}(\Omega)$. Therefore, it follows from $\varphi_1^1(x) = \varphi_1^2(x)$ that

$$\nabla T^1(x,t_1)\cdot\nu(x) = \nabla T^2(x,t_1)\cdot\nu(x), \quad T^1(x,t_1) = T^2(x,t_1), \quad x \in \partial\Omega$$

noticing that $\partial\Omega \in C^{2+l}$. Consequently, from $T^1(x,t_1) \ge T_0 > 0$ on $\partial\Omega$, the above equation leads to $(\alpha_1(x) - \alpha_2(x))T^1(x,t_1) = 0$, which yields $\alpha_1(x) = \alpha_2(x) = \alpha(x)$ for $x \in \partial\Omega$.

Now we prove the uniqueness for $q(x)$ by considering the inverse heat transfer problem in the time-layer $[t_1, t_f]$, given by

$$\begin{cases} \dfrac{\partial T^i}{\partial t}(x,t) - \nabla\cdot(k(x)\nabla T^i(x,t)) + q^i(x)T^i(x,t) = f(x,t), & (x,t) \in \Omega\times(t_1,t_f) =: Q_f, \\ k(x)\dfrac{\partial T^i}{\partial\nu} + \alpha(x)T^i(x,t) = \mu(x,t), & (x,t) \in \partial\Omega\times[t_1,t_f] =: S_f, \\ T^i(x,t_1) = \varphi_1(x), & x \in \overline{\Omega}, \end{cases} \tag{2.5}$$

with the extra data

$$T^i(x,t_f) = \varphi_2^i(x), \quad x \in \Omega. \tag{2.6}$$

At this stage, it is worth noting that the uniqueness of the potential $q(x)$ in the inverse problem (2.5) and (2.6) was established in [11] in the case when $\alpha = \mu = 0$, and in [13] in the case when $\varphi_1 = 0$. Below we give the proof of the more general situation of (2.5) and (2.6) without these particularisations.

We need to prove that $q^1(x) = q^2(x)$ from

$$(\varphi_1^1(x), \varphi_2^1(x)) = (\varphi_1^2(x), \varphi_2^2(x)) =: (\varphi_1(x), \varphi_2(x))$$

in terms of (2.5) and (2.6), which is equivalent to prove that the nonlinear equation

$$T[q](x, t_f) = \varphi_2(x), \quad x \in \Omega \tag{2.7}$$

has a unique solution $q(x) \in \mathcal{Q}$, where $T[q](x,t)$ is the solution to the problem

$$\begin{cases} \dfrac{\partial T}{\partial t}(x,t) - \nabla \cdot (k(x) \nabla T(x,t)) + q(x) T(x,t) = f(x,t), & (x,t) \in Q_f, \\ k(x) \dfrac{\partial T}{\partial \nu} + \alpha(x) T(x,t) = \mu(x,t), & (x,t) \in S_f, \\ T(x, t_1) = \varphi_1(x), & x \in \overline{\Omega}, \end{cases} \tag{2.8}$$

where the known initial condition $\varphi_1(x) = T(x, t_1) > T_0 > 0$ from the max-min principle noticing that $T(x, 0) = \varphi(x) > 0$ in Ω.

We apply the techniques used in [11] for a homogeneous Neumann boundary condition to establish the unique solvability of equation (2.7). Consider the mapping $\mathcal{U} : \mathcal{Q} \mapsto C^l(\Omega)$ defined by

$$\mathcal{U}[q](x) := q(x) + \Lambda(T[q](x, t_f) - \varphi_2(x)) \tag{2.9}$$

for $q \in \mathcal{Q}$, noticing that from the regularity of the solution of (2.8), $T[q](\cdot, t_f), \varphi_2(\cdot) \in C^{2+l}(\Omega) \subset C^l(\Omega)$. In (2.9), $\Lambda > 0$ is a constant whose value we are free to choose. If the mapping $\mathcal{U}$ has a fixed point $q \in \mathcal{Q}$, then we obtain $T[q](x, t_f) = \varphi_2(x)$, namely, q solves (2.7). Conversely, $q(x)$ must be a fixed point of the mapping $\mathcal{U}$ if $q \in \mathcal{Q}$ is the solution to (2.7). Due to this equivalence, the uniqueness of the solution to (2.7), is equivalent to the uniqueness of the fixed point of functional $\mathcal{U}[q]$ for any fixed constant $\Lambda > 0$.

Since $\mathcal{U} : \mathcal{Q} \mapsto C^l(\Omega)$ with $\mathcal{Q}$ being a closed non-negative cone of $C^l(\Omega)$, we can estimate both q and $\mathcal{U}[q]$ for $q \in \mathcal{Q}$ by the $C(\Omega)$ norm instead of $C^l(\Omega)$ norm. Assume that $q^1, q^2 \in \mathcal{Q}$ are two fixed points of functional $\mathcal{U}[q]$. If the nonlinear functional $\mathcal{U}[q]$ is strictly contractive in $\mathcal{Q}$ by $C(\Omega)$ norm, namely,

$$\|\mathcal{U}[z^1] - \mathcal{U}[z^2]\|_{C(\Omega)} \leq \beta \|z^1 - z^2\|_{C(\Omega)}, \quad \forall z^1, z^2 \in \mathcal{Q} \tag{2.10}$$

for some $\beta \in (0, 1)$, then the uniqueness of the fixed point of $\mathcal{U}[q]$ follows immediately from

$$\|q^1 - q^2\|_{C(\Omega)} = \|\mathcal{U}[q^1] - \mathcal{U}[q^2]\|_{C(\Omega)} \leq \beta \|q^1 - q^2\|_{C(\Omega)},$$

i.e., $q^1(x) = q^2(x) = q(x)$ in $C(\Omega)$. However, we also have the regularity $q^1(x), q^2(x) \in C^l(\Omega)$, so it follows that $q(x)$ is in $C^l(\Omega)$, i.e., $q(x)$ is in $\mathcal{Q}$.

To prove (2.10), from the mean value theorem for Gâteaux derivatives (see [52], p.13) we have that $\mathcal{U}[q]$ is strictly contractive in $\mathcal{Q}$ is equivalent to the contractiveness of the linear operator $\mathcal{U}'[q]$ on $\mathcal{Q}$ for any $q \in \mathcal{Q}$. So, we need to prove that for any fixed $q \in \mathcal{Q}$,

$$\|\mathcal{U}'[q] \diamond h\|_{C(\Omega)} \leq \beta^* \|h\|_{C(\Omega)}, \quad \forall h \in \mathcal{Q} \tag{2.11}$$

for some $\beta^* \in (0,1)$. By (2.9), we have

$$(\mathcal{U}'[q] \diamond h)(x) = h(x) - \Lambda\, (T'[q] \diamond h)(x, t_f), \quad x \in \Omega,$$

where $(T'[q] \diamond h)(x,t) := \hat{T}(x,t)$ is a linear functional of $h(x)$ satisfying

$$\begin{cases} \dfrac{\partial \hat{T}}{\partial t}(x,t) - \nabla \cdot (k \nabla \hat{T}(x,t)) + q(x)\hat{T}(x,t) = h(x)T[q](x,t), & (x,t) \in Q_f, \\ k(x)\dfrac{\partial \hat{T}}{\partial \nu} + \alpha(x)\hat{T} = 0, & (x,t) \in S_f, \\ \hat{T}(x,t_1) = 0, & x \in \overline{\Omega}. \end{cases} \tag{2.12}$$

Using the maximum principle, from $h(x)T[q](x,t) \geq q^- T_0 > 0$ and the comparison theorem, we have that $\hat{T}(x,t_f) \geq T^* > 0$ for some positive T^* which depends on q^- and T_0. So, the estimate (2.4) for the problem (2.12) yields

$$\begin{aligned} T^* \leq \hat{T}(x,t_f) &\leq \max_{(x,t)\in Q_f} \hat{T}(x,t) = \max_{(x,t)\in Q_f} |\hat{T}(x,t)| = \|\hat{T}\|_{C(Q_f)} \\ &\leq \|\hat{T}\|_{C^{2+l,1+l/2}(Q_f)} \leq c\|hT\|_{C^{l,l/2}(Q_f)} \leq c\|h\|_{C(\Omega)}\|T\|_{C^{l,l/2}(Q_f)} \leq cq^+\|T\|_{C^{l,l/2}(Q_f)} \end{aligned}$$

uniformly for all $x \in \Omega$, leading to $0 < q^- - c\Lambda\, q^+\|T\|_{C^{l,l/2}(Q_f)} \leq h(x) - \Lambda\,\hat{T}(x,t_f)$ for $\Lambda > 0$ small enough. Consequently,

$$\begin{aligned} \|(\mathcal{U}'[q] \diamond h)\|_{C(\Omega)} &= \sup_{x\in\Omega}(h(x) - \Lambda\,(T'[q]\diamond h)(x,t_f)) \leq \sup_{x\in\Omega}(h(x) - \Lambda\, T^*) \\ &= \|h\|_{C(\Omega)} - \Lambda\, T^* \leq \left(1 - \Lambda\, T^* \frac{1}{q^+}\right)\|h\|_{C(\Omega)} \end{aligned}$$

which leads to (2.11) with $\beta^* := \left(1 - \Lambda\, T^* \dfrac{1}{q^+}\right) \in (0,1)$ for $\Lambda > 0$ small enough.

Once the uniqueness of $q(x)$ and $\alpha(x)$ have been proven, now we can prove the uniqueness of initial temperature $\varphi(x)$ by considering the BHCP in the time-layer $[0,t_1]$ given by

$$\begin{cases} \dfrac{\partial T}{\partial t}(x,t) - \nabla \cdot (k(x)\nabla T(x,t)) + q(x)T(x,t) = f(x,t), & (x,t) \in \Omega \times (0,t_1) =: Q_1, \\ k(x)\dfrac{\partial T}{\partial \nu} + \alpha(x)T(x,t) = \mu(x,t), & (x,t) \in \partial\Omega \times [0,t_1] =: S_1, \\ T(x,t_1) = \varphi_1(x), & x \in \overline{\Omega}. \end{cases} \tag{2.13}$$

Assume the problem (2.13) has two solutions T^1 and T^2 and denote by $\tilde{T} = T^1 - T^2$ their difference which satisfies the problem

$$\begin{cases} \dfrac{\partial \tilde{T}}{\partial t}(x,t) - \nabla \cdot (k(x)\nabla \tilde{T}(x,t)) + q(x)\tilde{T}(x,t) = 0, & (x,t) \in Q_1, \\ k(x)\dfrac{\partial \tilde{T}}{\partial \nu} + \alpha(x)\tilde{T}(x,t) = 0, & (x,t) \in S_1, \\ \tilde{T}(x,t_1) = 0, & x \in \overline{\Omega}. \end{cases} \tag{2.14}$$

Denoted by $\{(\lambda_n, \psi_n[k,q,\alpha](x)) : n \in \mathbb{N}^*\}$ the orthogonal eigenpair system of the elliptic problem

$$\begin{cases} -\nabla \cdot (k(x)\nabla\psi) + q(x)\psi = \lambda\psi, & x \in \Omega, \\ k(x)\dfrac{\partial \psi}{\partial \nu} + \alpha(x)\psi = 0, & x \in \partial\Omega. \end{cases}$$

Then, the solution of the problem (2.14) can be represented as

$$\tilde{T}(x,t) = \sum_{n=1}^{\infty} c_n e^{-\lambda_n t} \psi_n[k,q,\alpha](x), \quad (x,t) \in \overline{\Omega} \times (0,t_1]. \tag{2.15}$$

Applying (2.15) at $t = t_1$ and using that $\tilde{T}(x,t_1) = 0$, it is easy to see that $c_n = 0$, $n \in \mathbb{N}^*$, which implies that $\tilde{T}(x,t) = 0$, in $L^2((0,t_1); H^1(\Omega))$. From (2.14) multiplying with $\tilde{T}$ and integrating, we obtain

$$\frac{1}{2}\int_{\Omega} |\tilde{T}(x,0)|^2 dx = \int_{Q_1} \left(k|\nabla \tilde{T}|^2 + q|\tilde{T}|^2 \right) dxdt + \int_{S_1} \alpha |\tilde{T}|^2 dsdt.$$

Since $q \in \mathcal{Q}$, $\alpha \in \mathcal{A}$ and $0 < k_0 \le k \in C^{1+l}(\Omega)$ we have the classical energy estimates, see also [53],

$$\int_{Q_1} \left(k|\nabla \tilde{T}|^2 + q|\tilde{T}|^2 \right) dxdt + \int_{S_1} \alpha |\tilde{T}|^2 dsdt \le c(k,q,\alpha) \|\tilde{T}\|^2_{L^2((0,t_1);H^1(\Omega))} = 0,$$

which implies that $\tilde{T}(x,0) = 0$ in $L^2(\Omega)$. Furthermore, due to the a-prior regularity of $\varphi \in \Phi$ it also follows that $\tilde{T}(x,0) = 0$ in the $C(\Omega)$ norm as well. The proof of Theorem 1 is complete. □

3. Optimization version for noisy input data

In terms of the proof scheme in the above section, the unique reconstruction of $\alpha(x)$ for $x \in \partial\Omega$, $q(x)$ and $\varphi(x)$ for $x \in \Omega$, together with the temperature $T(x,t)$ for $(x,t) \in Q$, from specified temperatures (2.2) at two instants t_1 and t_f is implemented by the following three steps:

- Step 1: Recover $\alpha(x)$ on $\partial\Omega$ using the compatibility between either conditions in (2.2) and the Robin boundary condition in (2.1) on $\partial\Omega$ at either $t = t_1$ or $t = t_f$, to formally obtain

$$\begin{aligned} &\alpha(x) = (\mu(x,t_1) - k(x)\nabla\varphi_1(x) \cdot \nu(x))/\varphi_1(x) \text{ or} \\ &\alpha(x) = (\mu(x,t_f) - k(x)\nabla\varphi_2(x) \cdot \nu(x))/\varphi_2(x), \quad x \in \partial\Omega; \end{aligned} \tag{3.1}$$

- Step 2: With $\alpha(x)$ on $\partial\Omega$ already determined in S1, recover the solution $(q(x), T(x,t))$ satisfying the inverse problem (see (2.5) and (2.6))

$$\begin{cases} \dfrac{\partial T}{\partial t}(x,t) - \nabla \cdot (k(x)\nabla T(x,t)) + q(x)T(x,t) = f(x,t), & (x,t) \in Q_f, \\ k(x)\dfrac{\partial T}{\partial \nu} + \alpha(x)T(x,t) = \mu(x,t), & (x,t) \in S_f, \\ T(x,t_1) = \varphi_1(x), \quad T(x,t_f) = \varphi_2(x), & x \in \overline{\Omega}; \end{cases} \tag{3.2}$$

- Step 3: With $\alpha(x)$ on $\partial\Omega$ and $q(x)$ in Ω already determined in Steps 1 and 2, respectively, recover the solution $(\varphi(x), T(x,t))$ of the BHCP given by (2.13).

Although the above reconstruction process, which recovers three unknowns step by step, is theoretically clear for the uniqueness, the numerical implementation is not so easy, since the reconstruction error in one step will contaminate the recovery in the next step. Especially, the realisation of Step 1 is based on the stable computation of the derivative $k\nabla\varphi_1 \cdot \nu$ or $k\nabla\varphi_2 \cdot \nu$ on $\partial\Omega$ from the noisy data (2.3), which has been previously studied thoroughly by one of the authors together with error analysis in [53]. Step 2 is the most challenging since the inverse problem is both nonlinear and ill-posed, whilst Step 3 considers a linear BHCP which has been investigated in many studies but which is still challenging due to its severe ill-posedness and heterogeneity of the material properties which are space-dependent.

In the following, we reconstruct $q(x)$ and $\varphi(x)$ simultaneously for known $\alpha(x)$ using the noisy data $(\varphi_1^\delta(x), \varphi_2^\delta(x))$. To deal with these noisy situations, we reformulate the inverse problem in its optimization version. Let $T(x,t;q,\varphi)$ be the solution of the direct problem (2.1). Introduce the admissible sets

$$\begin{aligned}\mathcal{A}_1 &= \{q \in L^\infty(\Omega) : 0 < q^- \le q(x) \le q^+,\ \text{a.e. } x \in \Omega\},\\ \mathcal{A}_2 &= \{\varphi \in L^2(\Omega) : 0 \le \varphi(x) \le F_0,\ \text{a.e. } x \in \Omega\}.\end{aligned}$$

The quasi-solution of the inverse problem is obtained by minimizing the Tikhonov-type objective functional $J[q,\varphi] : \mathcal{A}_1 \times \mathcal{A}_2 \to \mathbb{R}_+$ defined by

$$J[q,\varphi] = \frac{1}{2}\left(\|T(\cdot,t_1;q,\varphi) - \varphi_1^\delta(\cdot)\|^2_{L^2(\Omega)} + \|T(\cdot,t_f;q,\varphi) - \varphi_2^\delta(\cdot)\|^2_{L^2(\Omega)}\right) + \frac{\beta_1}{2}\|q\|^2_{L^2(\Omega)} + \frac{\beta_2}{2}\|\varphi\|^2_{L^2(\Omega)}, \tag{3.3}$$

where $\beta_1,\ \beta_2 > 0$ are regularization parameters to be prescribed and $T(x,t;q,\varphi) \in H^{1,0}(Q)$ is the weak solution to (2.1) satisfying the variational form

$$\begin{aligned}&\int_Q \left(-T\frac{\partial \eta}{\partial t} + (k\nabla T)\cdot\nabla\eta + qT\eta\right)dxdt + \int_S \alpha T\eta dsdt\\ =\ &\int_Q f\eta dxdt + \int_S \mu\eta dsdt + \int_\Omega \varphi\eta(x,0)dx, \quad \forall \eta \in H^{1,1}(Q),\ \eta(\cdot,t_f) = 0.\end{aligned} \tag{3.4}$$

The existence and uniqueness of $T(q,\varphi) \in H^{1,0}(Q)$ satisfying (3.4) for the direct problem (2.1) can be found in [54]. Moreover,

$$\|T\|_{H^{1,0}(Q)} + \max_{t\in[0,t_f]}\|T(\cdot,t)\|_{L^2(\Omega)} \le c\left(\|f\|_{L^2(Q)} + \|\mu\|_{L^2(S)} + \|\varphi\|_{L^2(\Omega)}\right) \tag{3.5}$$

for some constant $c > 0$ independent of f, μ and φ.

Inspired by the approaches in [33, 35, 55], the existence of a minimizer for the objective functional (3.3) over the admissible set $\mathcal{A}_1 \times \mathcal{A}_2$ is established as follows, for regularization parameters $\beta_1, \beta_2 > 0$ prescribed in advance.

Theorem 2. *There exists at least one minimizer to the optimization problem* (3.3) *and* (3.4)*.*

Proof. Since $\inf_{\mathcal{A}_1\times\mathcal{A}_2} J[q,\varphi] =: J_0 \ge 0$, there exists a minimizing sequence $\{(q^n,\varphi^n) : n \in \mathbb{N}\} \subset \mathcal{A}_1 \times \mathcal{A}_2$ such that

$$\lim_{n\to\infty} J[q^n,\varphi^n] = J_0,$$

which implies that $\{(q^n,\varphi^n) : n \in \mathbb{N}\}$ is uniformly bounded in $L^\infty(\Omega)\times L^2(\Omega)$ and thus there exists a subsequence, still denoted by $\{q^n,\varphi^n\}$, such that $(q^n,\varphi^n) \rightharpoonup (q^*,\varphi^*)$ in $L^\infty(\Omega)\times L^2(\Omega)$ with $(q^*,\phi^*) \in \mathcal{A}_1\times\mathcal{A}_2$. The *a-priori* estimate (3.5) implies that the sequence $\{T^n := T(q^n,\varphi^n) : n \in \mathbb{N}\}$ is uniformly bounded in $H^{1,0}(Q)$, noticing that the constant c depends only on q^+. Thus we may extract a subsequence, still denoted by $\{T^n : n \in \mathbb{N}\}$ such that $T^n \rightharpoonup T^* \in H^{1,0}(Q)$ in $H^{1,0}(Q)$.

From the definition (3.4) of the weak solution, for any $\eta \in H^{1,1}(Q)$ with $\eta(\cdot,t_f) = 0$, we have

$$\int_Q \left(-T^n\frac{\partial \eta}{\partial t} + (k\nabla T^n)\cdot\nabla\eta + q^nT^n\eta\right) + \int_S \alpha T^n\eta = \int_Q f\eta + \int_S \mu\eta + \int_\Omega \varphi^n\eta(x,0). \tag{3.6}$$

The third term in the left-hand side of (3.6) can be rewritten as

$$\int_Q q^n T^n \eta = \int_Q q^* T^n \eta + \int_Q (q^n - q^*) T^n \eta.$$

Since $q^n \rightharpoonup q^*$ in $L^\infty(\Omega)$, using the estimate (3.5) for T^n and the Lebesgue dominant convergence theorem giving $\int_Q (q^n - q) T^n \eta dxdt \to 0$, finally (3.6) leads to

$$\int_Q \left(-T^* \frac{\partial \eta}{\partial t} + (k \nabla T^*) \cdot \nabla \eta + q^* T^* \eta \right) + \int_S \alpha T^* \eta = \int_Q f \eta + \int_S \mu \eta + \int_\Omega \varphi^* \eta(x,0),$$

by $T^n \rightharpoonup T^*$ in $H^{1,0}(Q)$, $H^{1,0}(Q) \hookrightarrow L^2(Q)$ compactly, and $T^n|_S \rightharpoonup T^*|_S$ in $L^2(S)$.

Thus, we have $T^* = T(q^*, \varphi^*)$ due to the uniqueness of weak solution to direct problem (2.1). Now the lower semi-continuity of norms implies

$$\begin{aligned} J[q^*, \varphi^*] &= \frac{1}{2} \left(\|T^*(\cdot, t_1) - \varphi_1^\delta(\cdot)\|^2_{L^2(\Omega)} + \|T^*(\cdot, t_f) - \varphi_2^\delta(\cdot)\|^2_{L^2(\Omega)} \right) + \frac{\beta_1}{2} \|q^*\|^2_{L^2(\Omega)} + \frac{\beta_2}{2} \|\varphi^*\|^2_{L^2(\Omega)} \\ &\leq \frac{1}{2} \lim_{n \to \infty} \left(\|T^n(\cdot, t_1) - \varphi_1^\delta(\cdot)\|^2_{L^2(\Omega)} + \|T^n(\cdot, t_f) - \varphi_2^\delta(\cdot)\|^2_{L^2(\Omega)} \right) \\ &\quad + \frac{1}{2} \liminf_{n \to \infty} \left(\beta_1 \|q^n\|^2_{L^2(\Omega)} + \beta_2 \|\varphi^n\|^2_{L^2(\Omega)} \right) \\ &\leq \liminf_{n \to \infty} J[q^n, \varphi^n] = \inf_{\mathcal{A}_1 \times \mathcal{A}_2} J[q, \varphi], \end{aligned}$$

i.e., $\{q^*, \varphi^*\}$ is a minimizer of the optimization problem over $\mathcal{A}_1 \times \mathcal{A}_2$. The proof is complete. □

To find the minimizer, we will apply the CGM, where the gradient of $J[q, \varphi]$ is required. Consequently, we need to prove the differentiability of $T[q, \varphi]$, which is assisted by the following lemma.

Lemma 2. *The mapping $(q, \varphi) \mapsto T(q, \varphi)$ is Lipschitz continuous from $\mathcal{A}_1$ to $H^{1,0}(Q)$ with respect to q, and from $\mathcal{A}_2$ to $H^{1,0}(Q)$ with respect to φ, i.e.,*

$$\|T(q + \Delta q, \varphi) - T(q, \varphi)\|_{H^{1,0}(Q)} \leq c \|\Delta q\|_{L^\infty(\Omega)}, \tag{3.7}$$

$$\|T(q, \varphi + \Delta \varphi) - T(q, \varphi)\|_{H^{1,0}(Q)} \leq c \|\Delta \varphi\|_{L^2(\Omega)} \tag{3.8}$$

for any $q, q + \Delta q \in \mathcal{A}_1$, $\varphi, \varphi + \Delta \varphi \in \mathcal{A}_2$ and the corresponding $T(q, \varphi), T(q + \Delta q, \varphi), T(q, \varphi + \Delta \varphi) \in H^{1,0}(Q)$, where the constant $c = c(k, q^+, F_0)$.

Proof. The proof is just a straightforward application of (3.5) to the initial boundary value problems for $\Delta T_q := T(q + \Delta q, \varphi) - T(q, \varphi)$ and $\Delta T_\varphi := T(q, \varphi + \Delta \varphi) - T(q, \varphi)$. We omit the details. □

Based on the above lemma, now we can prove the differentiability of $T(q, \varphi)$.

Theorem 3. *The mapping $(q, \varphi) \mapsto T(q, \varphi)$ is Fréchet differentiable with respect to q and φ, i.e., there exist two bounded linear operators $\mathcal{U}_q : \mathcal{A}_1 \mapsto H^{1,0}(Q)$ and $\mathcal{U}_\varphi : \mathcal{A}_2 \mapsto H^{1,0}(Q)$ such that*

$$\lim_{\|\Delta q\|_{L^\infty(\Omega)} \to 0} \frac{\|T(q + \Delta q, \varphi) - T(q, \varphi) - \mathcal{U}_q \Delta q\|_{H^{1,0}(Q)}}{\|\Delta q\|_{L^\infty(\Omega)}} = 0, \tag{3.9}$$

$$\lim_{\|\Delta \varphi\|_{L^2(\Omega)} \to 0} \frac{\|T(q, \varphi + \Delta \varphi) - T(q, \varphi) - \mathcal{U}_\varphi \Delta \varphi\|_{H^{1,0}(Q)}}{\|\Delta \varphi\|_{L^2(\Omega)}} = 0. \tag{3.10}$$

Proof. For given $q \in \mathcal{A}_1$, consider the problem

$$\begin{cases} \dfrac{\partial u_q}{\partial t} = \nabla \cdot (k \nabla u_q) - q u_q - \Delta q T(q, \varphi), & (x,t) \in Q, \\ k(x) \dfrac{\partial u_q}{\partial \nu} + \alpha(x) u_q = 0, & (x,t) \in S, \\ u_q(x, 0) = 0, & x \in \overline{\Omega}, \end{cases} \tag{3.11}$$

for $\Delta q \in L^\infty(\Omega)$ such that $q + \Delta q \in \mathcal{A}_1$, where $T(q, \varphi)$ is the solution to direct problem (2.1). Then, there exists a unique solution $u_q(x,t) \in H^{1,0}(Q)$ for (3.11) depending on Δq linearly, and by (3.5), the mapping $\Delta q \mapsto u_q$, which is denoted by $\mathcal{U}_q$, is from $L^\infty(\Omega)$ to $H^{1,0}(Q)$.

Define $w_q := T(q + \Delta q, \varphi) - T(q, \varphi) - \mathcal{U}_q \Delta q = \Delta T_q - u_q$. Then, it is easy to verify that ΔT_q satisfies the problem

$$\begin{cases} \dfrac{\partial (\Delta T_q)}{\partial t} = \nabla \cdot (k \nabla (\Delta T_q)) - q \Delta T_q - \Delta q (\Delta T_q + T(q, \varphi)), & (x,t) \in Q, \\ k(x) \dfrac{\partial (\Delta T_q)}{\partial \nu} + \alpha(x) \Delta T_q = 0, & (x,t) \in S, \\ \Delta T_q(x, 0) = 0, & x \in \overline{\Omega}. \end{cases} \tag{3.12}$$

Using (3.11), then w_q satisfies

$$\begin{cases} \dfrac{\partial w_q}{\partial t} = \nabla \cdot (k \nabla w_q) - q w_q - \Delta q \Delta T_q, & (x,t) \in Q, \\ k(x) \dfrac{\partial w_q}{\partial \nu} + \alpha(x) w_q = 0, & (x,t) \in S, \\ w_q(x, 0) = 0, & x \in \overline{\Omega}. \end{cases}$$

Applying (3.5) to this problem, we obtain

$$\|w_q\|_{H^{1,0}(Q)} \le c \|\Delta q \Delta T_q\|_{L^2(Q)} \le c \|\Delta q\|_{L^\infty(\Omega)} \|\Delta T_q\|_{L^2(Q)} \le c \|\Delta q\|_{L^\infty(\Omega)} \|\Delta T_q\|_{H^{1,0}(Q)},$$

Using (3.7) in Lemma 2, the above estimate leads to

$$\|T(q + \Delta q, \varphi) - T(q, \varphi) - \mathcal{U}_q \Delta q\|_{H^{1,0}(Q)} = \|w_q\|_{H^{1,0}(Q)} \le c \|\Delta q\|^2_{L^\infty(\Omega)}.$$

So, we have proved (3.9).

Similarly, the function $\Delta T_\varphi = T(q, \varphi + \Delta \varphi) - T(q, \varphi)$ satisfies the problem

$$\begin{cases} \dfrac{\partial \Delta T_\varphi}{\partial t} = \nabla \cdot (k \nabla (\Delta T_\varphi)) - q \Delta T_\varphi, & (x,t) \in Q, \\ k(x) \dfrac{\partial (\Delta T_\varphi)}{\partial \nu} + \alpha(x) \Delta T_\varphi = 0, & (x,t) \in S, \\ \Delta T_\varphi(x, 0) = \Delta \varphi(x), & x \in \overline{\Omega}, \end{cases} \tag{3.13}$$

which defines a linear operator $\mathcal{U}_\varphi$ associated to $\Delta \varphi$. Then, the relation (3.10) can be proved analogously. The proof is completed. ☐

Theorem 4. *The objective functional $J[q, \varphi]$ is Fréchet differentiable and its Fréchet derivatives $J'_q[q, \varphi]$ and $J'_\varphi[q, \varphi]$ are given by*

$$J'_q[q, \varphi] = -\int_0^{t_f} T(x,t) \lambda(x,t) dt + \beta_1 q(x), \quad x \in \Omega, \tag{3.14}$$

$$J'_\varphi[q, \varphi] = \lambda(x, 0) + \beta_2 \varphi(x), \quad x \in \Omega, \tag{3.15}$$

where λ satisfies the following adjoint problem:

$$\begin{cases} \dfrac{\partial \lambda}{\partial t} = -\nabla \cdot (k\nabla\lambda) + q\lambda \\ \qquad -(T(x,t_1;q,\varphi) - \varphi_1^\delta)\tilde{\delta}(t-t_1) - 2(T(x,t_f;q,\varphi) - \varphi_2^\delta)\tilde{\delta}(t-t_f), & (x,t) \in Q, \\ k(x)\dfrac{\partial \lambda}{\partial \nu} + \alpha(x)\lambda = 0, & (x,t) \in S, \\ \lambda(x,t_f) = 0, & x \in \overline{\Omega}, \end{cases} \tag{3.16}$$

where $\tilde{\delta}(\cdot)$ denotes the Dirac delta function.

Proof. Taking any $\Delta q \in L^\infty(\Omega)$ such that $q + \Delta q \in \mathcal{A}_1$, we have

$$\begin{aligned} & J[q+\Delta q,\varphi] - J[q,\varphi] \\ = \; & \frac{1}{2}\int_\Omega \left\{ \left[T(x,t_1;q+\Delta q,\varphi) - \varphi_1^\delta(x)\right]^2 + \left[T(x,t_f;q+\Delta q,\varphi) - \varphi_2^\delta(x)\right]^2 \right\} dx \\ & -\frac{1}{2}\int_\Omega \left\{ \left[T(x,t_1;q,\varphi) - \varphi_1^\delta(x)\right]^2 + \left[T(x,t_f;q,\varphi) - \varphi_2^\delta(x)\right]^2 \right\} dx + \frac{\beta_1}{2}\int_\Omega \left\{ (q+\Delta q)^2 - q^2 \right\} dx \\ = \; & \frac{1}{2}\|\Delta T_q(\cdot,t_1)\|^2_{L^2(\Omega)} + \int_Q \Delta T_q(x,t)\left[T(x,t_1;q,\varphi) - \varphi_1^\delta(x)\right]\tilde{\delta}(t-t_1)dxdt + \beta_1\int_\Omega q\Delta q dx \\ & +\frac{1}{2}\|\Delta T_q(\cdot,t_f)\|^2_{L^2(\Omega)} + 2\int_Q \Delta T_q(x,t)\left[T(x,t_f;q,\varphi) - \varphi_2^\delta(x)\right]\tilde{\delta}(t-t_f)dxdt + \frac{\beta_1}{2}\|\Delta q\|^2_{L^2(\Omega)}. \end{aligned}$$

Let λ be the weak solution of the problem (3.16). Integrating by parts in the above identity, we have

$$\begin{aligned} J[q+\Delta q,\varphi] - J[q,\varphi] &= \int_Q \Delta T_q \left\{ -\frac{\partial\lambda}{\partial t} - \nabla\cdot(k\nabla\lambda) + q\lambda \right\} dxdt \\ & +\beta_1\int_\Omega q\Delta q dx + \frac{\beta_1}{2}\|\Delta q\|^2_{L^2(\Omega)} + \frac{1}{2}\|\Delta T_q(\cdot,t_1)\|^2_{L^2(\Omega)} + \frac{1}{2}\|\Delta T_q(\cdot,t_f)\|^2_{L^2(\Omega)} \\ = \; & \int_Q \lambda\left\{ \frac{\partial(\Delta T_q)}{\partial t} - \nabla\cdot(k\nabla(\Delta T_q)) + q\Delta T_q \right\} dxdt - \int_\Omega \Delta T_q \lambda|_0^{t_f} dx \\ & + \int_S \left(k\frac{\partial(\Delta T_q)}{\partial\nu}\lambda - k\frac{\partial\lambda}{\partial\nu}\Delta T_q \right) dsdt + \beta_1\int_\Omega q\Delta q dx + \frac{\beta_1}{2}\|\Delta q\|^2_{L^2(\Omega)} \\ & +\frac{1}{2}\|\Delta T_q(\cdot,t_1)\|^2_{L^2(\Omega)} + \frac{1}{2}\|\Delta T_q(\cdot,t_f)\|^2_{L^2(\Omega)} \\ = \; & -\int_Q \Delta q T(q+\Delta q,\varphi)\lambda dxdt + \beta_1\int_\Omega q\Delta q dx + \frac{\beta_1}{2}\|\Delta q\|^2_{L^2(\Omega)} \\ & +\frac{1}{2}\|\Delta T_q(\cdot,t_1)\|^2_{L^2(\Omega)} + \frac{1}{2}\|\Delta T_q(\cdot,t_f)\|^2_{L^2(\Omega)}. \end{aligned}$$

Using (3.5), (3.7) and (3.12) we have

$$\max\left\{\|\Delta T_q(\cdot,t_1)\|^2_{L^2(\Omega)}, \|\Delta T_q(\cdot,t_f)\|^2_{L^2(\Omega)}\right\} \le \max_{t\in[0,t_f]}\|\Delta T_q(\cdot,t)\|^2_{L^2(\Omega)} \le c\|T\|^2_{L^2(Q)}\|\Delta q\|^2_{L^\infty(\Omega)},$$

$$\left| \int_Q \Delta q \Delta T_q \lambda dxdt \right| \le \|\Delta q\|_{L^\infty(\Omega)}\|\Delta T_q\|_{L^2(Q)}\|\lambda\|_{L^2(Q)} \le c\|\Delta q\|^2_{L^\infty(\Omega)}\|\lambda\|_{L^2(Q)}.$$

Using these estimates in

$$-\int_Q \Delta q T(q+\Delta q,\varphi)\lambda dxdt = -\int_Q \Delta q \Delta T_q \lambda dxdt - \int_Q \Delta q T\lambda dxdt,$$

we obtain that

$$J[q+\Delta q,\varphi]-J[q,\varphi] = -\int_Q \Delta q T\lambda dxdt + \int_\Omega \beta_1 q\Delta q dx + o(\|\Delta q\|_{L^\infty(\Omega)}),$$

which means that the Fréchet derivative $J'_q[q,\varphi]$ is given by (3.14).

Using a similar approach, we obtain

$$J[q,\varphi+\Delta\varphi]-J[q,\varphi] = \int_\Omega \Delta\varphi(\lambda(x,0)+\beta_2\varphi)dx + o(\|\Delta\varphi\|_{L^2(\Omega)}),$$

thus the Fréchet derivative $J'_\varphi[q,\varphi]$ is given by (3.15). The proof is completed. □

Note that the Fréchet gradients $J'_q[q,\varphi]$, $J'_\varphi[q,\varphi]$ and the adjoint problem (3.16) will be utilized in the nonlinear CGM for the reconstruction of the unknown coefficients (q,φ) in the inverse problem (3.3) and (3.4) in the next section.

4. Conjugate gradient method

The following iterative process based on the CGM is now used for the estimation of $q(x)$ and $\varphi(x)$ by minimizing the objective functional $J[q,\varphi]$:

$$q^{n+1}(x) = q^n(x) - \beta_q^n P_q^n(x), \quad n=0,1,2,\cdots, \tag{4.1}$$

$$\varphi^{n+1}(x) = \varphi^n(x) - \beta_\varphi^n P_\varphi^n(x), \quad n=0,1,2,\cdots, \tag{4.2}$$

where n denotes the number of iterations, $q^0(x)$ and $\varphi^0(x)$ are the initial guesses for $q(x)$ and $\varphi(x)$, β_q^n and β_φ^n are the step search sizes for $q(x)$ and $\varphi(x)$ in passing from iteration n to iteration $n+1$, and $P_q^n(x)$ and $P_\varphi^n(x)$ are the directions of descent given by

$$P_q^0 = J'_q[q^0,\varphi^0], \quad P_q^n = J'_q[q^n,\varphi^n] + \gamma_q^n P_q^{n-1}, \quad n=1,2,\cdots, \tag{4.3}$$

$$P_\varphi^0 = J'_\varphi[q^0,\varphi^0], \quad P_\varphi^n = J'_\varphi[q^n,\varphi^n] + \gamma_\varphi^n P_\varphi^{n-1}, \quad n=1,2,\cdots \tag{4.4}$$

Different expressions are available for the conjugate coefficients γ_q^n and γ_φ^n, e.g., for the Fletcher–Reeves method [23, 56, 57],

$$\gamma_q^n = \frac{\|J'_q[q^n,\varphi^n]\|^2_{L^2(\Omega)}}{\|J'_q[q^{n-1},\varphi^{n-1}]\|^2_{L^2(\Omega)}}, \quad n=1,2,\cdots, \tag{4.5}$$

$$\gamma_\varphi^n = \frac{\|J'_\varphi[q^n,\varphi^n]\|^2_{L^2(\Omega)}}{\|J'_\varphi[q^{n-1},\varphi^{n-1}]\|^2_{L^2(\Omega)}}, \quad n=1,2,\cdots \tag{4.6}$$

The search step sizes β_q^n and β_φ^n are found by minimizing

$$\begin{aligned}J[q^{n+1},\varphi^{n+1}] =& \frac{1}{2}\int_\Omega [T(x,t_1;q^n-\beta_q^nP_q^n,\varphi^n-\beta_\varphi^nP_\varphi^n)-\varphi_1^\delta(x)]^2dx + \frac{\beta_1}{2}\int_\Omega (q^n-\beta_q^nP_q^n)^2dx\\ &+\frac{1}{2}\int_\Omega [T(x,t_f;q^n-\beta_q^nP_q^n,\varphi^n-\beta_\varphi^nP_\varphi^n)-\varphi_2^\delta(x)]^2dx + \frac{\beta_2}{2}\int_\Omega (\varphi^n-\beta_\varphi^nP_\varphi^n)^2dx.\end{aligned}$$

Setting $\Delta q^n = P_q^n$ and $\Delta\varphi^n = P_\varphi^n$, the estimated temperature $T(x,t_1;q^n-\beta_q^n P_q^n,\varphi^n-\beta_\varphi^n P_\varphi^n)$ and $T(x,t_f;q^n-\beta_q^n P_q^n,\varphi^n-\beta_\varphi^n P_\varphi^n)$ are linearised by a Taylor series expansion in the form

$$\begin{aligned}T(x,t';q^n-\beta_q^n P_q^n,\varphi^n-\beta_\varphi^n P_\varphi^n) &\approx T(x,t';q^n,\varphi^n)-\beta_q^n P_q^n\frac{\partial T(x,t';q^n,\varphi^n)}{\partial q^n}-\beta_\varphi^n P_\varphi^n\frac{\partial T(x,t';q^n,\varphi^n)}{\partial\varphi^n}\\ &\approx T(x,t';q^n,\varphi^n)-\beta_q^n\Delta T_q(x,t';q^n,\varphi^n)-\beta_\varphi^n\Delta T_\varphi(x,t';q^n,\varphi^n)\end{aligned}$$

where t' represents t_1 and t_f, respectively.

Then, denoting $T_1^n = T(x,t_1;q^n,\varphi^n)$, $T_f^n = T(x,t_f;q^n,\varphi^n)$, $\Delta T_{q,1}^n = \Delta T_q(x,t_1;q^n,\varphi^n)$, $\Delta T_{q,f}^n = \Delta T_q(x,t_f;q^n,\varphi^n)$, $\Delta T_{\varphi,1}^n = \Delta T_\varphi(x,t_1;q^n,\varphi^n)$ and $\Delta T_{\varphi,f}^n = \Delta T_\varphi(x,t_f;q^n,\varphi^n)$, we have

$$\begin{aligned}J[q^{n+1},\varphi^{n+1}] =&\frac{1}{2}\int_\Omega[T_1^n-\beta_q^n\Delta T_{q,1}^n-\beta_\varphi^n\Delta T_{\varphi,1}^n-\varphi_1^\delta(x)]^2dx+\frac{\beta_1}{2}\int_\Omega(q^n-\beta_q^n P_q^n)^2dx\\ &+\frac{1}{2}\int_\Omega[T_f^n-\beta_q^n\Delta T_{q,f}^n-\beta_\varphi^n\Delta T_{\varphi,f}^n-\varphi_2^\delta(x)]^2dx+\frac{\beta_2}{2}\int_\Omega(\varphi^n-\beta_\varphi^n P_\varphi^n)^2dx.\end{aligned}$$

We calculate the partial derivatives with respect to β_q^n and β_φ^n to obtain

$$\frac{\partial J}{\partial\beta_q^n}=C_1\beta_q^n+C_2\beta_\varphi^n-C_3,\quad \frac{\partial J}{\partial\beta_\varphi^n}=C_2\beta_q^n+C_4\beta_\varphi^n-C_5,$$

where

$$\begin{aligned}C_1&=\int_\Omega\left[(\Delta T_{q,1}^n)^2+(\Delta T_{q,f}^n)^2+\beta_1(P_q^n)^2\right]dx,\quad C_2=\int_\Omega\left(\Delta T_{q,1}^n\Delta T_{\varphi,1}^n+\Delta T_{q,f}^n\Delta T_{\varphi,f}^n\right)dx,\\ C_3&=\int_\Omega\left[(T_1^n-\varphi_1^\delta)\Delta T_{q,1}^n+(T_f^n-\varphi_2^\delta)\Delta T_{q,f}^n+\beta_1 q^n P_q^n\right]dx,\\ C_4&=\int_\Omega\left[(\Delta T_{\varphi,1}^n)^2+(\Delta T_{\varphi,f}^n)^2+\beta_2(P_\varphi^n)^2\right]dx,\\ C_5&=\int_\Omega\left[(T_1^n-\varphi_1^\delta)\Delta T_{\varphi,1}^n+(T_f^n-\varphi_2^\delta)\Delta T_{\varphi,f}^n+\beta_2\varphi^n P_\varphi^n\right]dx.\end{aligned}$$

Next, we set $\dfrac{\partial J}{\partial\beta_q^n}=\dfrac{\partial J}{\partial\beta_\varphi^n}=0$, and obtain the search step sizes β_q^n and β_φ^n as follows:

$$\beta_q^n=\frac{C_2C_5-C_3C_4}{C_2^2-C_1C_4},\quad \beta_\varphi^n=\frac{C_2C_3-C_1C_5}{C_2^2-C_1C_4},\quad n=0,1,\cdots \tag{4.7}$$

When $\beta_1=\beta_2=0$, the unregularized iterative procedure given by equations (4.1) and (4.2) does not provide the CGM with the stabilization necessary for the minimization of the function (3.3) to be classified as well-posed because of the errors in the measurements (2.2). However, the CGM becomes well-posed if the discrepancy principle is used to stop the iterative procedure when

$$J[q^n,\varphi^n]\approx\frac{1}{2}\left(\|\varphi_1^\delta-\varphi_1\|^2_{L^2(\Omega)}+\|\varphi_2^\delta-\varphi_2\|^2_{L^2(\Omega)}\right). \tag{4.8}$$

To summarise, the steps of the CGM for reconstructing the unknown space-dependent coefficients $q(x)$ and $\varphi(x)$, are as follows:

S1 Set $n=0$ and choose initial guesses $q^0(x)$ and $\varphi^0(x)$ for the unknowns $q(x)$ and $\varphi(x)$, respectively.

S2 Solve the direct problem (2.1) (using e.g., the finite-difference method (FDM)) to compute $T(x, t; q^n, \varphi^n)$ and $J[q^n, \varphi^n]$.

S3 Solve the adjoint problem (3.16) to compute the Lagrange multiplier $\lambda(x, t; q^n, \varphi^n)$, and the gradients $J'_q[q^n, \varphi^n]$ in (3.14) and $J'_\varphi[q^n, \varphi^n]$ in (3.15). Compute the conjugate coefficients γ_q^n and γ_φ^n in (4.5) and (4.6), and the directions of descent P_q^n and P_φ^n in (4.3) and (4.4).

S4 Solve the sensitivity problems (3.12) and (3.13) to compute the functions $\Delta T_q(x, t; q^n, \varphi^n)$ and $\Delta T_\varphi(x, t; q^n, \varphi^n)$ by taking $\Delta q^n(x) = P_q^n(x)$ and $\Delta\varphi^n(x) = P_\varphi^n(x)$, and compute the search step sizes β_q^n and β_φ^n in (4.7).

S5 Compute q^{n+1} and φ^{n+1} by (4.1) and (4.2). In case q^{n+1} takes negative values replace it by $\max\{0, q^{n+1}\}$ in order to enforce the physical constraint that the coefficient $q(x)$ cannot be negative.

S6 When $\beta_1 = \beta_2 = 0$, the stopping condition is: If the condition (4.8) is satisfied, then go to S7. Else set $n = n + 1$, and go to S2.

S7 End.

Remark 2. *(i) At this stage it is worth mentioning that another possible approach, motivated by [58], was also developed based on decoupling the simultaneous identification into first obtaining the domain HTC $q(x)$ using the CGM [21] by solving the inverse coefficient problem in the region $\Omega \times (t_1, t_f)$, after which the initial temperature $\varphi(x)$ is obtained using an elliptic approximation method [26] for solving the BHCP in the region $\Omega \times (0, t_1)$. However, due to the uncontrollable noise present or accumulated in $q(x)$, $\varphi_1(x)$ and $\partial_t T(x, t_1)$, which are needed as input in this latter operator splitting method, the numerically obtained results were rather inconsistent and therefore they are not presented.*
(ii) Compared to other related methods of minimization [18, 19, 20], the CGM is expected to perform equally well in terms of accuracy and stability, with the extra feature of being faster, since the step search sizes β_q^n and β_φ^n in (4.1) and (4.2), respectively, are optimized as in (4.7). However, this comparison is deferred to a future work.

5. Numerical results and discussions

In this section we show the numerical results for the initial temperature $\varphi(x)$ and the domain HTC $q(x)$ reconstructed simultaneously by the nonlinear CGM, as described in Section 4. As described before at the beginning of Section 3, the surface HTC, $\alpha(x)$, is assumed to have been separately/independently obtained, prior to the simultaneous inversion of $(q(x), \varphi(x))$, using the formal expression (3.1) in case of exact input data (2.2), or the regularization techniques described in [53] in case of noise data (2.3).

The FDM based on the Crank-Nicolson scheme in one-dimension $N = 1$, and the alternating direction implicit (ADI) scheme in two-dimensions $N = 2$, [21], are employed to solve the direct, sensitivity and adjoint problems. Note that the source term in (3.16) contains the Dirac delta function which is approximated by

$$\delta_a(t - t_i) \approx \frac{1}{a\sqrt{\pi}} e^{-(t-t_i)^2/a^2}, \quad i = 1, f, \tag{5.1}$$

where a is a small positive constant taken as $a = 10^{-3}$. The Simpson's rule is used to approximate all the integrals involved. We define the errors at the iteration number n for $q(x)$ and $\varphi(x)$ as

$$E_1[q^n] = \|q - q^n\|_{L^2(\Omega)}, \tag{5.2}$$
$$E_2[\varphi^n] = \|\varphi - \varphi^n\|_{L^2(\Omega)}. \tag{5.3}$$

The temperature measurement φ_1^δ at time t_1 and the final temperature measurement φ_2^δ at time t_f containing random noise are simulated by adding to the exact data φ_1 and φ_2 error terms generated from a normal distribution in the following forms:

$$\varphi_1^\delta = \varphi_1 + \sigma \times \text{random}(1), \quad \varphi_2^\delta = \varphi_2 + \sigma \times \text{random}(1), \tag{5.4}$$

where $\sigma = \dfrac{p}{100} \times \max_{x\in\overline{\Omega}}\{|\varphi_1(x)|, |\varphi_2(x)|\}$, $p\%$ represents the percentage of noise, and random(1) generates random values from the normal distribution with mean equal to 0 and standard deviation equal to unity using MATLAB.

At this stage, we note that the CGM regularization can be accomplished either by including regularization with appropriate positive regularization parameters β_1 and β_2 in (3.3), and running for all iterations n until there is no significant difference between consecutive iterates or, in the case $\beta_1 = \beta_2 = 0$, stopping the iterations according to the discrepancy principle (4.8). However, as demonstrated in [59] for a linear sideways heat conduction problem, there is no significant difference in the numerical results obtained by these approaches. Therefore, in this section we only present the numerical results obtained by taking $\beta_1 = \beta_2 = 0$ in (3.3), which becomes

$$J_0[q, \varphi] := \frac{1}{2}\left(\|T(\cdot, t_1; q, \varphi) - \varphi_1^\delta\|^2_{L^2(\Omega)} + \|T(\cdot, t_f; q, \varphi) - \varphi_2^\delta\|^2_{L^2(\Omega)}\right), \tag{5.5}$$

and employ the stopping criterion (4.8).

5.1. Example 1

In the one-dimensional case we take $\Omega = (0, 1)$. We also take $t_1 = 0.5$, $t_f = 1$ and

$$k \equiv 1, \quad f(x,t) = x(1 + 2x + x^2)e^{-t}, \quad \mu(0,t) = e^{-t}, \quad \mu(1,t) = 4e^{-t}, \tag{5.6}$$
$$\varphi_1(x) = e^{-0.5}(1 + x^2), \quad \varphi_2(x) = e^{-1}(1 + x^2). \tag{5.7}$$

Then the analytical solution of the inverse problem is

$$\alpha(x) = 1, \quad x \in \partial\Omega, \quad q(x) = 3 + x, \quad \varphi(x) = 1 + x^2, \quad x \in \Omega, \tag{5.8}$$
$$T(x,t) = e^{-t}(1 + x^2), \quad (x,t) \in \Omega \times (0, t_f). \tag{5.9}$$

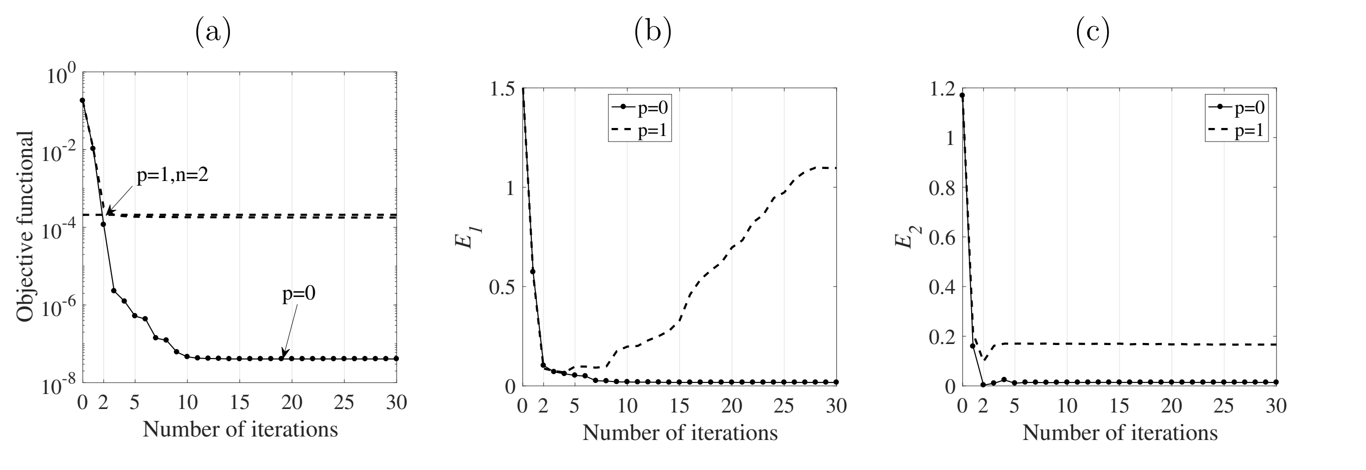

Figure 2: (a) The objective functional (5.5), the errors (b) (5.2) and (c) (5.3), for $p \in \{0, 1\}$ noise, for Example 1.

For obtaining the components $q(x)$, $\varphi(x)$ and $T(x,t)$ of the solution we use the FDM Crank-Nicolson scheme with mesh sizes $\Delta x = \Delta t = 0.025$ to solve the PDEs involved in the CGM. In this example, the initial guesses q^0 and φ^0 for $q(x)$ and $\varphi(x)$ are chosen as $q^0(x) = 2$ and $\varphi^0(x) = x+2$.

In Figures 2(a)–2(c), the objective functional $J_0[q^n, \varphi^n]$ given by (5.5), and the errors $E_1[q^n]$ given by (5.2) and $E_2[\varphi^n]$ given by (5.3) are illustrated for the simultaneous numerical reconstruction of the initial temperature $\varphi(x)$ and the domain HTC $q(x)$ using the CGM of Section 4. Figure 2(a) shows the monotonic decreasing convergence of the objective functional (5.5), as a function of the number of iterations n, for $p \in \{0, 1\}$ noise. The stopping number for the iterations is 30 for no noise $p = 0$, and 2 iterations according to the discrepancy principle (4.8) for $p = 1$ noise. These values are in good agreement with the optimal values of the iteration numbers, which can be inferred from Figures 2(b) and 2(c) included herein only for illustrative purposes.

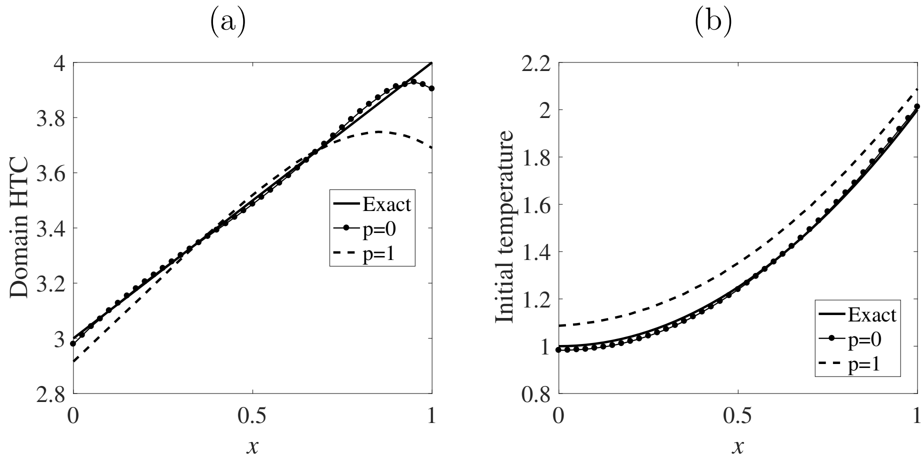

Figure 3: The exact and numerical results for (a) the domain HTC $q(x)$ and (b) the initial temperature $\varphi(x)$, for $p \in \{0, 1\}$ noise, for Example 1.

The corresponding numerical solutions for $q(x)$ and $\varphi(x)$ are shown in Figures 3(a) and 3(b), respectively. First, it can be seen that in the case of no noise, the retrieved solutions for both the domain HTC $q(x)$ and the initial temperature $\varphi(x)$ are in very good agreement ($E_1[q^{30}] = 0.0174$, $E_2[\varphi^{30}] = 0.0139$) with the exact solutions (5.8). Second, in the case of noisy data $p = 1$, the retrieved solutions are stable and also in reasonable agreement ($E_1[q^2] = 0.0875$, $E_2[\varphi^2] = 0.0985$) with the exact solutions (5.8) for both functions.

5.2. Example 2

The previous example has been concerned with the recovery of smooth functions in (5.8). In this example, we investigate a more severe situation in which the domain HTC in (5.13) is a discontinuous function. We take $\Omega = (0, 1)$, $t_1 = 0.5$, $t_f = 1$ and

$$k \equiv 1, \quad \mu(0,t) = \mu(1,t) = e^{-t},$$

$$f(x,t) = \pi^2 \sin(\pi x) e^{-t} + (1 + \pi + \sin(\pi x)) e^{-t} \times \begin{cases} 1 - x, & x \in [0, 0.3], \\ -x + 4x^2, & x \in (0.3, 0.7), \\ 2, & x \in [0.7, 1], \end{cases} \tag{5.10}$$

$$\varphi_1(x) = e^{-0.5}(1 + \pi + \sin(\pi x)), \quad \varphi_2(x) = e^{-1}(1 + \pi + \sin(\pi x)). \tag{5.11}$$

Then the analytical solution of the inverse problem is

$$\alpha(x) = 1, \quad T(x,t) = (1 + \pi + \sin(\pi x))e^{-t}, \quad \varphi(x) = 1 + \pi + \sin(\pi x), \tag{5.12}$$

$$q(x) = \begin{cases} 2 - x, & x \in [0, 0.3], \\ 1 - x + 4x^2, & x \in (0.3, 0.7), \\ 3, & x \in [0.7, 1]. \end{cases} \tag{5.13}$$

The initial guesses are chosen as $q^0(x) = 1$ and $\varphi^0(x) = 2$ for the two unknowns $q(x)$ and $\varphi(x)$, respectively. The FDM Crank-Nicolson scheme with the mesh sizes $\Delta x = \Delta t = 0.01$ is utilized to solve the PDEs involved in the CGM.

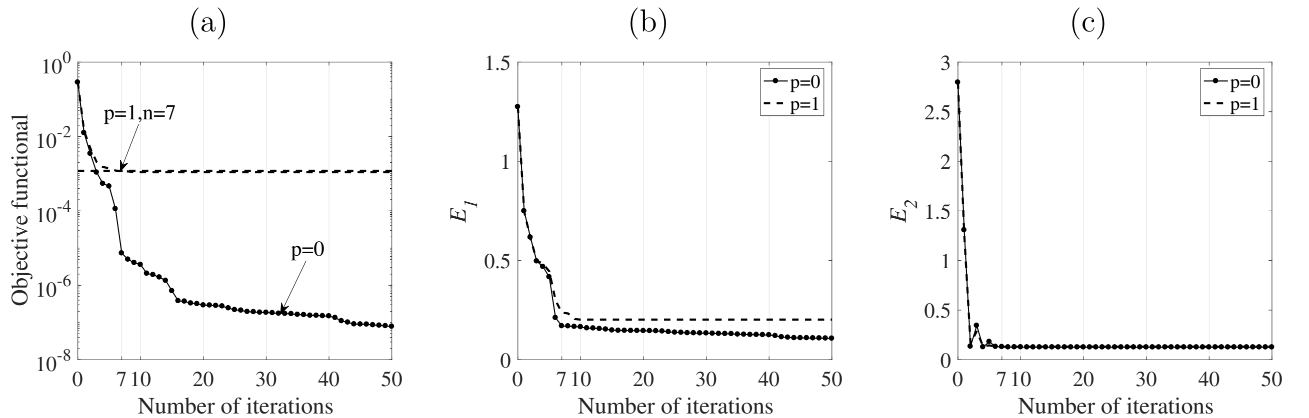

Figure 4: (a) The objective functional (5.5), the errors (b) (5.2) and (c) (5.3), for $p \in \{0, 1\}$ noise, for Example 2.

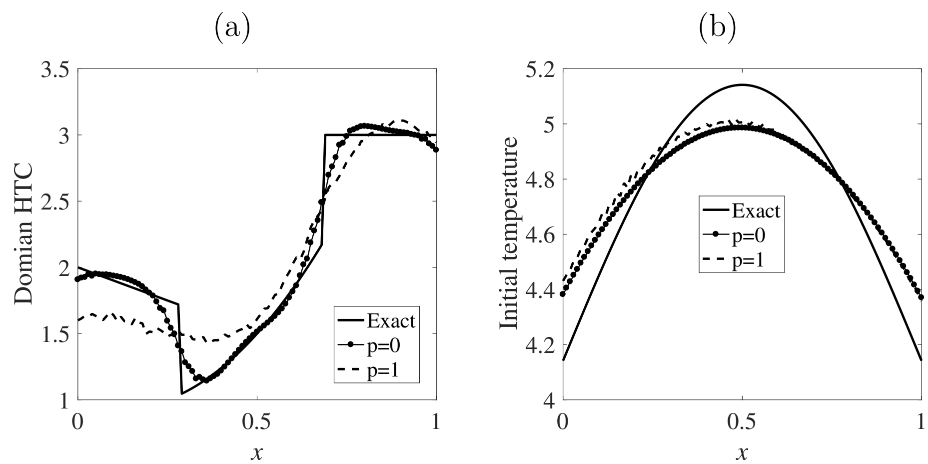

Figure 5: The exact and numerical results for (a) the domain HTC $q(x)$ and (b) the initial temperature $\varphi(x)$, for $p \in \{0, 1\}$ noise, for Example 2.

The objective functional $J_0[q^n, \varphi^n]$ given by (5.5), and the errors $E_1[q^n]$ given by (5.2) and $E_2[\varphi^n]$ given by (5.3), illustrated in Figures 4(a)-4(c), for $p \in \{0, 1\}$ noise, present similar features to those in Figures 2(a)–2(c) for Example 1. The corresponding numerical results for $q(x)$ and $\varphi(x)$ are illustrated in Figures 5(a) and 5(b), respectively. We also quantify the errors (5.2) and (5.3), as given by $E_1[q^{30}] = 0.1072$, $E_2[\varphi^{30}] = 0.1260$ for $p = 0$, and $E_1[q^7] = 0.2372$, $E_2[\varphi^7] = 0.1309$ for $p = 1$. From these errors and Figure 5 it can be concluded that the numerical solutions are stable and reasonably accurate bearing in mind the difficult discontinuous domain HTC $q(x)$ in (5.13) that had to be retrieved.

5.3. *Example 3*

In the two-dimensional case we take $\Omega = (0,1) \times (0,1)$. We also take $t_1 = 0.5$, $t_f = 1$ and

$$k = \mathbf{I}_2, \quad f(x_1,x_2,t) = (4+x_1+x_2)(1+x_1^2+x_2^2)e^{-t} - 4e^{-t}, \quad \mu(0,x_2,t) = (1+x_2^2)e^{-t},$$

$$\mu(1,x_2,t) = (4+x_2^2)e^{-t}, \quad \mu(x_1,0,t) = (1+x_1^2)e^{-t}, \quad \mu(x_1,1,t) = (4+x_1^2)e^{-t}, \tag{5.14}$$

$$\varphi_1(x_1,x_2) = e^{-0.5}(1+x_1^2+x_2^2), \quad \varphi_2(x_1,x_2) = e^{-1}(1+x_1^2+x_2^2). \tag{5.15}$$

The analytical solution of the inverse problem is given by

$$\alpha(x_1,x_2) = 1, \quad q(x_1,x_2) = 5+x_1+x_2, \quad \varphi(x_1,x_2) = 1+x_1^2+x_2^2, \tag{5.16}$$

$$T(x_1,x_2,t) = (1+x_1^2+x_2^2)e^{-t}. \tag{5.17}$$

We employ the ADI scheme with mesh sizes $\Delta x_1 = \Delta x_2 = \Delta t = 0.05$ to solve the PDEs involved in the CGM, with the initial guesses $q^0(x_1,x_2) = 4$ and $\varphi^0(x_1,x_2) = 1.5 + x_1 + x_2$.

The objective functional (5.5), the accuracy errors (5.2) and (5.3), and the exact (5.16) and numerical solutions for the two unknown functions $q(x_1,x_2)$ and $\varphi(x_1,x_2)$, obtained using the CGM of Section 4 are shown in Figures 6–8. Similar conclusions to those drawn from Figures 2 and 3 of Example 1 can be made. According to Figure 6(a), and further argued in Figures 6(b) and 6(c), the iterations are stopped after 30 for $p=0$ and 4 for $p=1$, giving the errors (5.2) and (5.3) from Figures 7 and 8 as $E_1[q^{30}] = 0.0886$, $E_2[\varphi^{30}] = 0.0336$ for $p=0$, and $E_1[q^4] = 0.1117$, $E_2[\varphi^4] = 0.0454$ for $p=1$.

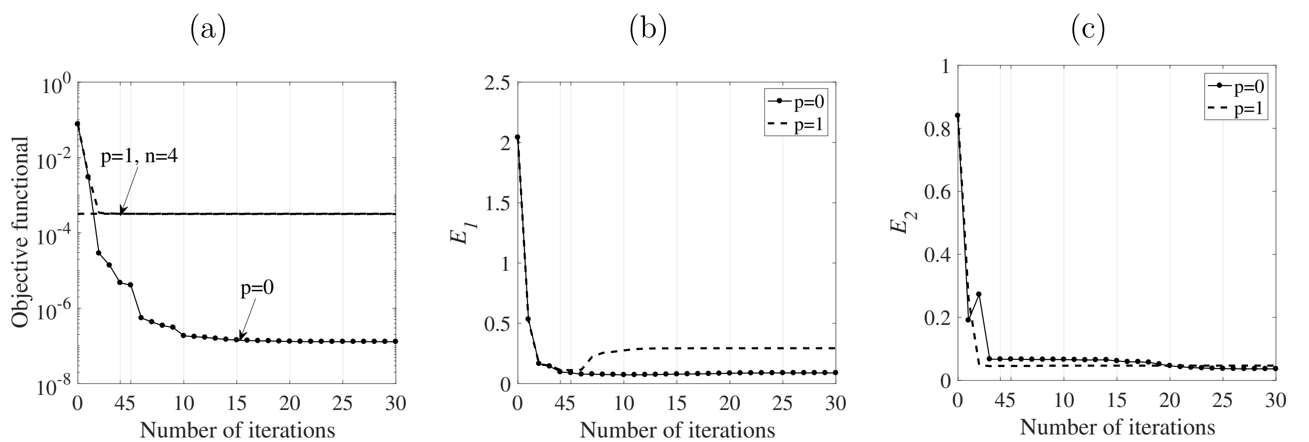

Figure 6: (a) The objective functional (5.5), the errors (b) (5.2) and (c) (5.3), for $p \in \{0,1\}$ noise, for Example 3.

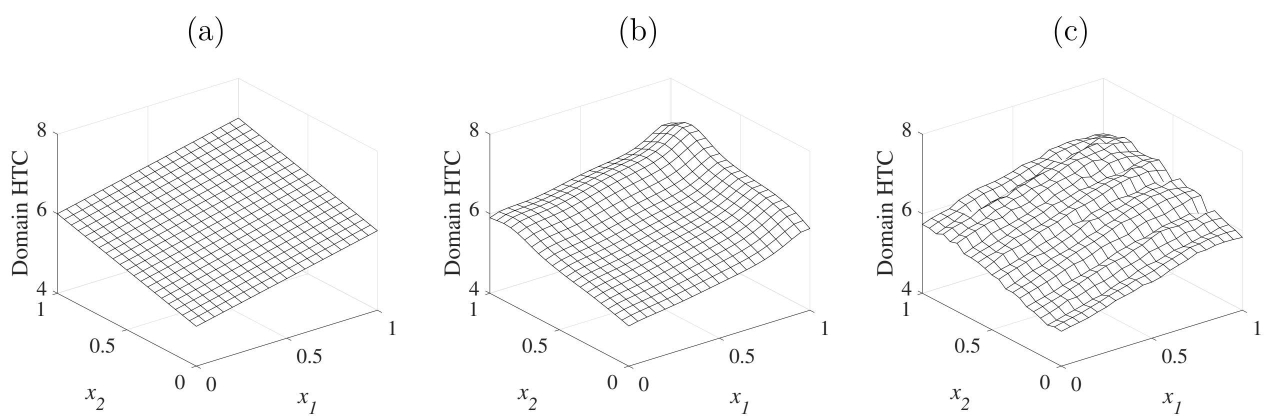

Figure 7: (a) The exact and numerical results for $q(x_1,x_2)$ for (b) $p=0$ and (c) $p=1$ noise, for Example 3.

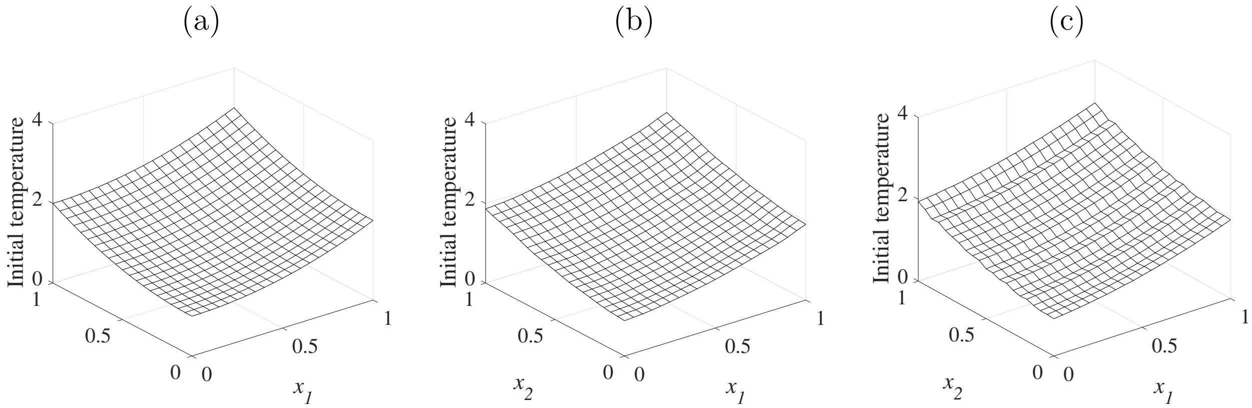

Figure 8: (a) The exact and numerical results for $\varphi(x_1, x_2)$ for (b) $p = 0$ and (c) $p = 1$ noise, for Example 3.

6. Conclusions

The analysis of this paper has successfully pushed the boundaries of inverse problem formulations to a different level of challenge by simultaneously reconstructing the space-dependent surface and domain HTCs along with the initial temperature from temperature measurements at two different instants. The interior transient temperature inside the solution domain, at the boundary and the heat flux are also obtained as a by-product of solving the problem. The uniqueness of the HTCs and the initial temperature in the inverse problem have been proved rigorously. With the already determined surface HTC, the remaining two unknown functions have been simultaneously reconstructed by minimizing a Tikhonov-type objective functional. The existence of a minimizer of the objective functional has been proved, and the Fréchet gradients have been obtained by a variational method. Then, the CGM has been applied to simultaneously determine the two unknown quantities. Three numerical experiments for one- and two-dimensional examples have been illustrated and discussed. Good accuracy and reasonable stability have been achieved. Nevertheless, there is a need in the future to utilise the analysis of this paper to promote the benefits of the proposed inverse mathematical model by conducting industrial trials and inversion of raw temperature data.

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