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Simultaneous reconstruction of the spatially-distributed reaction coefficient, initial temperature and heat source from temperature measurements at different times

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Abstract

In many practical situations concerned with high temperatures/pressures/loads and/or hostile environments, certain properties of the physical medium, geometry, boundary and/or initial conditions are not known and their direct measurement can be very inaccurate or even inaccessible. In such situations, one can adopt an inverse approach and try to infer the unknowns from some extra accessible measurements of other quantities that may be available. However, the simultaneous identification of several non-constant physical properties along with initial and/or boundary conditions is very challenging, especially when it cannot be decoupled, as it combines both nonlinear as well as ill-posedness features. One such new inverse problem concerning the identification of the space-dependent reaction coefficient, the initial temperature and the source term from measured temperatures at two instants t_1, t_2 and at the final time T, where $0 < t_1 < t_2 < T$, is investigated in this paper. Insight into the uniqueness of solution is gained by considering various particular cases. Moreover, as in practice the input temperature data are usually noise polluted due to the errors that are inherently present, their influence on the solution of inversion has to be assessed. As such, the least-squares objective functional modelling the gap between the measured and computed data is minimized to obtain the quasi-solution to the inverse problem, and the Fréchet gradients are obtained. The conjugate gradient method (CGM) with the Fletcher-Reeves formula is applied to estimate the three unknown coefficients numerically. Numerical examples are illustrated to show that accurate and stable numerical solutions are obtained using the CGM regularized by the discrepancy principle.

Keywords: inverse problem; parabolic equation; conjugated gradient method; initial temperature; reaction coefficient; heat source

1. Introduction

The complex modelling of heat transfer process 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]. Most of previous studies on inverse problems concerned determining a single unknown physical quantity. For instance, the nonlinear identification of the space-dependent reaction coefficient from final temperature observation was theoretically investigated in [2, 3, 4, 5], and numerically reconstructed using many numerical algorithms, such

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as the Armijo algorithm combined with the finite element method (FEM) [6], or the CGM with the finite-difference method (FDM) [7]. The linear identification of the space-dependent source term from temperature measurements at the final time was also widely studied, e.g., [8, 9, 10]. Finally, the backward heat conduction problem (BHCP) for the reconstruction of the initial temperature from measured temperature at a later time was extensively studied, e.g., using the CGM [11, 12], the boundary element method (BEM) with regularization [13], the BEM combined with an elliptic approximation [14], the Fourier regularization method [15], and the self-adaptive Lie-group method [16].

In [17, 18], the space-dependent reaction coefficient and the initial temperature were simultaneous identified from the final observation of temperature and the measured temperature in $\omega \times (0, T)$, where ω is a subregion of the space domain Ω. Also, in [19], the space-dependent heat source and the initial temperature were identified from temperature measurements of two distinct instants.

In this paper, the simultaneous reconstruction of the spatially-distributed reaction coefficient, the initial temperature, the heat source, and the temperature throughout the solution domain from temperature measurements at three different instants, is investigated for the first time. The least-squares objective functional, whose minimizer is proven to exist, is minimized to obtain a quasi-solution to the inverse problem. A variational method is applied to derive the Fréchet gradients subject to the three unknown coefficients together with the adjoint and sensitivity problems. The CGM [11, 20], which is established from the gradients, and the adjoint and sensitivity problems, are utilized to simultaneously reconstruct the three unknown functions. Furthermore, since the inverse problem is ill-posed, the CGM is regularized by the discrepancy principle [11] to obtain stable numerical results.

This paper is organized as follows: Section 2 presents the inverse problem to reconstruct the unknown space-dependent reaction coefficient, initial temperature and source term. The least-squares objective functional to be minimized is described having several properties in Section 3. The CGM is established in Section 4 based on the gradients of the objective functional, and the adjoint and sensitivity problems, and the global convergence for the CGM algorithm is obtained. Two numerical examples for the one-dimensional inverse problem are discussed in Section 5. Finally, Section 6 highlights the conclusions of this work.

2. Mathematical formulation and analysis

In the cylinder $Q := \Omega \times (0, T)$, where $\Omega \subset \mathbb{R}^N$, $(N = 1, 2, 3)$, is a bounded domain with a sufficient smooth boundary $\partial\Omega$, and $T > 0$ is a final time of interest, consider the heat transfer process governed by the parabolic equation

$$\frac{\partial u}{\partial t}(x,t) = \nabla \cdot (k(x)\nabla u(x,t)) - q(x)u(x,t) + F(x,t), \quad (x,t) \in Q, \tag{1}$$

where $u(x,t)$ is the temperature, k is the thermal conductivity, $q(x) \geq 0$ is the space-dependent reaction (radiative [17], perfusion [7], heat transfer) coefficient, $F(x,t)$ is the heat source term, and for simplicity the heat capacity has been taken to be unity. For the boundary condition we assume that this of Robin convection type

$$k(x)\frac{\partial u}{\partial \nu}(x,t) + \alpha(x)u(x,t) = \mu(x,t), \quad (x,t) \in S := \partial\Omega \times (0,T), \tag{2}$$

where ν is the outward unit normal to the boundary $\partial\Omega$, μ is a given heat flux function and $\alpha(x) \geq 0$ is the surface heat transfer coefficient. Condition (2) becomes the Neumann heat flux boundary condition when $\alpha(x) \equiv 0$.

At the initial time $t = 0$,

$$u(x,0) = \phi(x), \quad x \in \Omega, \tag{3}$$

denotes the initial temperature.

The space $L_2(\Omega)$ consists of all square-integrable functions $v(x)$ over Ω, endowed with the norm

$$\|v\|_{L_2(\Omega)} = \left(\int_\Omega |v(x)|^2 dx\right)^{1/2}.$$

The space $L_\infty(\Omega)$ comprises all essentially bounded functions $v(x)$ in Ω, equipped with the norm

$$\|v\|_{L_\infty(\Omega)} = \operatorname*{ess\,sup}_{x\in\Omega} |v(x)| := \inf\{M \geq 0 : |v(x)| \leq M, \text{ a.e. } x \in \Omega\}.$$

The spaces $L_2(Q)$ and $L_\infty(Q)$ can be defined similarly. We denote by $H^{1,0}(Q)$ the normed space of all functions $u(x,t) \in L_2(Q)$ having weak first-order derivatives with respect to x in $L_2(Q)$, endowed with the norm

$$\|u\|_{H^{1,0}(Q)} = \left(\|u\|^2_{L_2(Q)} + \|\nabla u\|^2_{L_2(Q)}\right)^{1/2}.$$

In the literature the space $H^{1,0}(Q)$ coincides with the space $L_2(0,T; H^1(\Omega))$ and with the Sobolev space $W_2^{1,0}(Q)$, ([21], p.138).

The space $H^{1,1}(Q)$, defined by $H^{1,1}(Q) = \left\{u \in L_2(Q) : \frac{\partial u}{\partial t} \text{ and } \nabla u \in L_2(Q)\right\}$, is a normed space with

$$\|u\|_{H^{1,1}(Q)} = \left(\|u\|^2_{L_2(Q)} + \|\nabla u\|^2_{L_2(Q)} + \|u_t\|^2_{L_2(Q)}\right)^{1/2},$$

where the gradient ∇ is with respect to x.

Throughout this work, we assume that the operator $\mathcal{L} := \frac{\partial}{\partial t} - \nabla \cdot (k\nabla) + q\mathcal{I}$, where $\mathcal{I}$ is the identical operator, is assumed to be uniformly parabolic, i.e., the matrix $(k_{ij})_{i,j=\overline{1,N}}$ is positive definite, namely,

$$\upsilon_1|\xi|^2 \leq \sum_{i,j=1}^N k_{ij}(x)\xi_i\xi_j \leq \upsilon_2|\xi|^2, \quad \text{a.e. } x \in \Omega,\ \forall\xi = (\xi_i)_{i=\overline{1,N}} \in \mathbb{R}^N, \tag{4}$$

for some given positive constants υ_1 and υ_2.

Definition 1. *A function $u \in H^{1,0}(Q)$ is called as a weak solution to the initial-boundary value direct problem* (1)–(3) *if*

$$\begin{aligned}&\int_Q \left(-u\frac{\partial \eta}{\partial t} + k\nabla u \cdot \nabla\eta + qu\eta\right) dxdt + \int_S \alpha u\eta dsdt \\ &= \int_Q F\eta dxdt + \int_S \mu\eta dsdt + \int_\Omega \phi\eta(\cdot,0)dx, \quad \forall\eta \in H^{1,1}(Q) \text{ with } \eta(\cdot,T) = 0.\end{aligned} \tag{5}$$

The existence and uniqueness of the weak solution to the initial-boundary value direct problem (1)–(3) is stated in the following theorem ([21], p.373).

Theorem 1. *Let $\Omega \subset \mathbb{R}^N$ be a bounded domain with Lipschitz boundary $\partial\Omega$, and suppose that the matrix $k = (k_{ij})_{i,j=\overline{1,N}}$ is symmetric and positive definite, i.e., $k_{ij} = k_{ji} \in L_\infty(\Omega)$ and satisfy (4), $q \in L_\infty(\Omega)$, $F \in L_2(Q)$, $\alpha \in L_\infty(\partial\Omega)$, $\mu \in L_2(S)$ and $\phi \in L_2(\Omega)$. Then the initial-boundary value direct problem (1)–(3) has a unique weak solution $u \in H^{1,0}(Q)$. In addition, the solution satisfies the estimate*

$$\max_{t\in[0,T]} \|u(\cdot,t)\|_{L_2(\Omega)} + \|u\|_{H^{1,0}(Q)} \leq c\left(\|F\|_{L_2(Q)} + \|\mu\|_{L_2(S)} + \|\phi\|_{L_2(\Omega)}\right) \tag{6}$$

for some positive constant $c(k,q,\alpha)$ which is independent of F, μ and ϕ.

For the inverse problem with an unknown heat source we suppose that the source term $F(x,t)$ has the form $F(x,t) = f(x)h(x,t) + g(x,t)$, such that (1) becomes

$$\frac{\partial u}{\partial t}(x,t) = \nabla\cdot(k(x)\nabla u(x,t)) - q(x)u(x,t) + f(x)h(x,t) + g(x,t), \quad (x,t)\in Q, \tag{7}$$

where $h \in L_\infty(Q)$, $g \in L_2(Q)$ are given functions and $f \in L_2(\Omega)$ is an unknown component of the heat source F. Then, the inverse problem is to reconstruct $(q(x),\phi(x),f(x),u(x,t)) \in L_\infty^+(\Omega) \times L_2(\Omega) \times L_2(\Omega) \times H^{1,0}(Q)$ satisfying (2) and (7) together with the temperature measurements at two time instants t_1, t_2, $0 < t_1 < t_2 < T$ and the final time T, namely,

$$u(x,t_1) = \phi_1(x), \quad x\in\Omega, \tag{8}$$
$$u(x,t_2) = \phi_2(x), \quad x\in\Omega, \tag{9}$$
$$u(x,T) = \phi_T(x), \quad x\in\Omega, \tag{10}$$

where $\phi_1(x)$, $\phi_2(x)$ and $\phi_T(x)$ are given data in $L_2(\Omega)$ which may be subject to noise due to measurement errors satisfying

$$\|\phi_1^\epsilon - \phi_1\|_{L_2(\Omega)} \leq \epsilon, \quad \|\phi_2^\epsilon - \phi_2\|_{L_2(\Omega)} \leq \epsilon, \quad \|\phi_T^\epsilon - \phi_T\|_{L_2(\Omega)} \leq \epsilon, \tag{11}$$

where $\epsilon \geq 0$ represents the noise level.

2.1. Discussion on the uniqueness of solution

Clearly, the initial temperature (3) can be uniquely retrieved by solving the BHCP in the layer $\Omega\times(0,t_1]$, if it would be the possible to establish separately the uniqueness for the triplet $(q(x),f(x),u(x,t))$ satisfying (2), (7)–(10) in the upper layer $\Omega\times[t_1,T]$, which includes the intermediate temperature measurement (9) at $t = t_2 \in (t_1,T)$. However, the uniqueness of solution of this latter, combined multiple coefficient nonlinear problem is more difficult, as described next. Ignoring for time being the regularity of the data and solution, let us proceed formally by first differentiating (2) and (7) with respect to t to obtain

$$\frac{\partial v}{\partial t}(x,t) = \nabla\cdot(k(x)\nabla v(x,t)) - q(x)v(x,t) + f(x)h_t(x,t) + g_t(x,t), \quad (x,t)\in Q, \tag{12}$$
$$k(x)\frac{\partial v}{\partial \nu}(x,t) + \alpha(x)v(x,t) = \mu_t(x,t), \quad (x,t)\in S, \tag{13}$$

where $v(x,t) := u_t(x,t)$. Conditions (8)–(10) also yield

$$\int_{t_1}^{t_2} v(x,t)dt = \phi_2(x) - \phi_1(x) =: \psi_1(x), \quad x\in\Omega, \tag{14}$$
$$\int_{t_2}^{T} v(x,t)dt = \phi_T(x) - \phi_2(x) =: \psi_2(x), \quad x\in\Omega. \tag{15}$$

If h is independent of t, then $h_t = 0$ and the unknown source f eliminates from (12). Then the resulting inverse problem for determining the reaction coefficient $q(x)$ and the temperature $u(x,t)$ becomes as given by equations (13)–(15) and

$$\frac{\partial v}{\partial t}(x,t) = \nabla \cdot (k(x)\nabla v(x,t)) - q(x)v(x,t) + g_t(x,t), \quad (x,t) \in Q, \tag{16}$$

which has recently been investigated by the authors in [22]. In particular, it is possible to eliminate $q(x)$ from (16) by integrating it from t_1 to t_2 and from t_2 to T and use (14) and (15) to result in the following quasi-direct problem for $v(x,t)$ (dropping, for simplicity, the known term $g_t(x,t)$ taken to be zero):

$$\begin{cases} \frac{\partial v}{\partial t}(x,t) = \nabla \cdot (k(x)\nabla v(x,t)) - v(x,t)\left(\frac{\nabla\cdot(k(x)\nabla\psi_2(x)) - v(x,T) + v(x,t_2)}{\psi_2(x)}\right), & (x,t) \in Q, \\ k(x)\frac{\partial v}{\partial \nu}(x,t) + \alpha(x)v(x,t) = \mu_t(x,t), & (x,t) \in S, \\ v(x,t_2) - v(x,t_1) = \nabla \cdot (k(x)\nabla\psi_1(x)) - \psi_1(x)\left(\frac{\nabla\cdot(k(x)\nabla\psi_2(x)) - v(x,T) + v(x,t_2)}{\psi_2(x)}\right), & x \in \Omega. \end{cases} \tag{17}$$

Problems of this type (17) were previously mentioned in [23] and considered in [24], but afterwards they have been somewhat overlooked in the literature.

In conclusion, the analysis of uniqueness of solution is still pending and subject to ongoing investigation, but nevertheless, it is still possible to develop a variational formulation for obtaining a quasi-solution, as described in the next section.

3. Variational formulation

Let $u(q,\phi,f) := u(x,t;q,\phi,f) \in H^{1,0}(Q)$ denote the solution to the initial-boundary value direct problem (1)–(3) for a particular triplet $(q(x),\phi(x),f(x)) \in L_\infty(\Omega) \times L_2(\Omega) \times L_2(\Omega)$. The quasi-solution of the inverse problem (2), (7)–(10) can be attained by minimizing the following least-squares objective functional

$$J(q,\phi,f) = \frac{1}{2}\left\{\|u_1 - \phi_1^\epsilon\|^2_{L_2(\Omega)} + \|u_2 - \phi_2^\epsilon\|^2_{L_2(\Omega)} + \|u_T - \phi_T^\epsilon\|^2_{L_2(\Omega)}\right\}, \tag{18}$$

where $u_1(x) = u(x,t_1;q,\phi,f)$, $u_2(x) = u(x,t_2;q,\phi,f)$ and $u_T(x) = u(x,T;q,\phi,f)$.

Let us define the sets

$$\mathcal{A}_1 = \{q \in L_\infty(\Omega) : 0 \le q(x) \le \kappa_1, \text{ a.e. } x \in \Omega\},$$

$$\mathcal{A}_2 = \{\phi \in L_2(\Omega) : |\phi(x)| \le \kappa_2, \text{ a.e. } x \in \Omega\}$$

and

$$\mathcal{A}_3 = \{f \in L_2(\Omega) : |f(x)| \le \kappa_3, \text{ a.e. } x \in \Omega\},$$

where κ_1, κ_2 and κ_3 are given positive constants. The existence of a minimizer to the optimization problem (18) over the admissible set $\mathcal{A}_1 \times \mathcal{A}_2 \times \mathcal{A}_3$ is established in the following theorem based on the approach utilized in [17, 25].

Theorem 2. *There exists at least one minimizer to the optimization problem* (18).

Proof. Based on the estimate (6), it is obvious that $\min J(q,\phi,f)$ is finite over the admissible set $\mathcal{A}_1\times\mathcal{A}_2\times\mathcal{A}_3$. Thus, there exists a minimizing sequence $\{q^n,\phi^n,f^n\}$ from $\mathcal{A}_1\times\mathcal{A}_2\times\mathcal{A}_3$ such that

$$\lim_{n\to\infty} J(q^n,\phi^n,f^n)=\inf_{q\in\mathcal{A}_1,\phi\in\mathcal{A}_2,f\in\mathcal{A}_3} J(q,\phi,f).$$

This implies the boundedness of $\{q^n,\phi^n,f^n\}$ in $L_\infty(\Omega)\times L_2(\Omega)\times L_2(\Omega)$, which yields that there exists a subsequence, still denoted by $\{q^n,\phi^n,f^n\}$, such that q^n, ϕ^n and f^n converge weakly to q^* in $L_\infty(\Omega)$, ϕ^* in $L_2(\Omega)$, and f^* in $L_2(\Omega)$. Clearly $q^*\in\mathcal{A}_1$, $\phi^*\in\mathcal{A}_2$ and $f^*\in\mathcal{A}_3$, since the sets $\mathcal{A}_1$, $\mathcal{A}_2$ and $\mathcal{A}_3$ are closed and convex. Then, Theorem 1 and the *a priori* estimate (6) imply that the sequence $\{u^n:=u(q^n,\phi^n,f^n)\}$ exists, is unique and is uniformly bounded in $H^{1,0}(Q)$. Thus, we can extract a subsequence, still denoted by $\{u^n\}$, and some $u^*\in H^{1,0}(Q)$ such that $u^n\to u^*$ weakly in $H^{1,0}(Q)$. Since $H^{1,0}(Q)|_S$ is compactly imbedded into $L_2(S)$, we obtain that $u^n|_S$ converges to $u^*|_S$ in $L_2(S)$, [26].

By Definition 1 and $F(x,t)=f(x)h(x,t)+g(x,t)$, for any $\eta\in H^{1,1}(Q)$ with $\eta(\cdot,T)=0$, we have

$$\begin{aligned}&\int_Q\left(-u^n\frac{\partial\eta}{\partial t}+k\nabla u^n\cdot\nabla\eta+q^nu^n\eta\right)dxdt+\int_S\alpha u^n\eta dsdt\\&=\int_Q f^nh\eta dxdt+\int_Q g\eta dxdt+\int_S\mu\eta dsdt+\int_\Omega\phi^n\eta(\cdot,0)dx.\end{aligned}\tag{19}$$

The weak convergence of u^n to u^* in $H^{1,0}(Q)$ and the convergence of $u^n|_S$ to $u^*|_S$ in $L_2(S)$ imply that

$$\begin{aligned}&\lim_{n\to\infty}\int_Q -u^n\frac{\partial\eta}{\partial t}dxdt=\int_Q -u^*\frac{\partial\eta}{\partial t}dxdt,\quad \lim_{n\to\infty}\int_Q k\nabla u^n\cdot\nabla\eta dxdt=\int_Q k\nabla u^*\cdot\nabla\eta dxdt,\\&\lim_{n\to\infty}\int_S\alpha u^n\eta dsdt=\int_S\alpha u^*\eta dsdt,\end{aligned}$$

and the weak convergence of ϕ^n to ϕ^* and f^n to f^* in $L_2(\Omega)$ implies that

$$\lim_{n\to\infty}\int_Q f^nh\eta dxdt=\int_Q f^*h\eta dxdt,\quad \lim_{n\to\infty}\int_\Omega\phi^n\eta(\cdot,0)dx=\int_\Omega\phi^*\eta(\cdot,0)dx.$$

The third term in the left hand side of (19) can be rewritten as

$$\int_Q q^nu^n\eta dxdt=\int_Q q^*u^n\eta dxdt+\int_Q(q^n-q^*)u^n\eta dxdt.$$

Since u^n weakly converges to u^* in $H^{1,0}(Q)$, we have $\lim_{n\to\infty}\int_Q q^*u^n\eta dxdt=\int_Q q^*u^*\eta dxdt$, and due to q^n weakly converges to q^* in $L_\infty(\Omega)$, using the estimate (6) for u^n and the Lebesgue dominant convergence theorem we obtain that the term $\int_Q(q^n-q^*)u^n\eta dxdt$ converges to zero, and hence

$$\lim_{n\to\infty}\int_Q q^nu^n\eta dxdt=\int_Q q^*u^*\eta dxdt,$$

and (19) yields

$$\begin{aligned}&\int_Q\left(-u^*\frac{\partial\eta}{\partial t}+(k\nabla u^*)\cdot\nabla\eta+q^*u^*\eta\right)dxdt+\int_S\alpha u^*\eta dsdt\\&=\int_Q f^*h\eta dxdt+\int_Q g\eta dxdt+\int_S\mu\eta dsdt+\int_\Omega\phi^*\eta(\cdot,0)dx,\end{aligned}$$

which means that $u^* = u(q^*, \phi^*, f^*)$, due to the uniqueness of solution to the initial-boundary value direct problem (1)–(3) in Theorem 1, with $q = q^*$, $f = f^*$ in (1), and $\phi = \phi^*$ in (3), respectively. The lower semi-continuity of norms implies

$$
\begin{aligned}
J(q^*, \phi^*, f^*) =& \frac{1}{2} \left\{ \|u_1^* - \phi_1^\epsilon\|^2_{L_2(\Omega)} + \|u_2^* - \phi_2^\epsilon\|^2_{L_2(\Omega)} + \|u_T^* - \phi_T^\epsilon\|^2_{L_2(\Omega)} \right\} \\
\leq& \frac{1}{2} \lim_{n\to\infty} \left\{ \|u_1^n - \phi_1^\epsilon\|^2_{L_2(\Omega)} + \|u_2^n - \phi_2^\epsilon\|^2_{L_2(\Omega)} + \|u_T^n - \phi_T^\epsilon\|^2_{L_2(\Omega)} \right\} \\
=& \lim_{n\to\infty} J(q^n, \phi^n, f^n) = \min_{q\in\mathcal{A}_1, \phi\in\mathcal{A}_2, f\in\mathcal{A}_3} J(q^n, \phi^n, f^n),
\end{aligned}
$$

which indicates that the triplet $\{q^*, \phi^*, f^*\}$ is a minimizer of the optimization problem (18) over $\mathcal{A}_1 \times \mathcal{A}_2 \times \mathcal{A}_3$. □

Lemma 1. *The mapping $(q, \phi, f) \mapsto u(q, \phi, f)$ from $L_\infty(\Omega) \times L_2(\Omega) \times L_2(\Omega)$ to $H^{1,0}(Q)$ is Lipschitz continuous, i.e.,*

$$
\|u(q + \Delta q, \phi, f) - u(q, \phi, f)\|_{H^{1,0}(Q)} \leq c\|\Delta q\|_{L_\infty(\Omega)}, \tag{20}
$$
$$
\|u(q, \phi + \Delta\phi, f) - u(q, \phi, f)\|_{H^{1,0}(Q)} \leq c\|\Delta \phi\|_{L_2(\Omega)}, \tag{21}
$$
$$
\|u(q, \phi, f + \Delta f) - u(q, \phi, f)\|_{H^{1,0}(Q)} \leq c\|\Delta f\|_{L_2(\Omega)}, \tag{22}
$$

for any $q, q + \Delta q \in \mathcal{A}_1$, $\phi, \phi + \Delta\phi \in \mathcal{A}_2$ and $f, f + \Delta f \in \mathcal{A}_3$. Moreover, the mapping is Fréchet differentiable.

Proof. Denote by $\Delta u_q = u(q + \Delta q, \phi, f) - u(q, \phi, f)$, $\Delta u_\phi = u(q, \phi + \Delta\phi, f) - u(q, \phi, f)$ and $\Delta u_f = u(q, \phi, f + \Delta f) - u(q, \phi, f)$ the increments of the temperature u with respect to q, ϕ and f. Then, based on the initial-boundary value problem (2), (3) and (7) they satisfy the following problems:

$$
\begin{cases}
\frac{\partial(\Delta u_q)}{\partial t} = \nabla \cdot (k\nabla(\Delta u_q)) - q\Delta u_q - \Delta q u(q + \Delta q, \phi, f), & (x, t) \in Q, \\
k\frac{\partial(\Delta u_q)}{\partial \nu} + \alpha \Delta u_q = 0, \quad (x, t) \in S, \quad \Delta u_q(x, 0) = 0, & x \in \overline{\Omega},
\end{cases} \tag{23}
$$

$$
\begin{cases}
\frac{\partial(\Delta u_\phi)}{\partial t} = \nabla \cdot (k\nabla(\Delta u_\phi)) - q\Delta u_\phi, & (x, t) \in Q, \\
k\frac{\partial(\Delta u_\phi)}{\partial \nu} + \alpha \Delta u_\phi = 0, \quad (x, t) \in S, \quad \Delta u_\phi(x, 0) = \Delta\phi, & x \in \overline{\Omega},
\end{cases} \tag{24}
$$

and

$$
\begin{cases}
\frac{\partial(\Delta u_f)}{\partial t} = \nabla \cdot (k\nabla(\Delta u_f)) - q\Delta u_f + \Delta f h, & (x, t) \in Q, \\
k\frac{\partial(\Delta u_f)}{\partial \nu} + \alpha \Delta u_f = 0, \quad (x, t) \in S, \quad \Delta u_f(x, 0) = 0, & x \in \overline{\Omega},
\end{cases} \tag{25}
$$

Using the *a priori* estimate (6) to the above problem, we obtain

$$
\begin{aligned}
&\|\Delta u_q\|_{H^{1,0}(Q)} \leq c\|\Delta q u\|_{L_2(Q)} \leq c\|\Delta q\|_{L_\infty(\Omega)}\|u\|_{L_2(Q)}, \\
&\|\Delta u_\phi\|_{H^{1,0}(Q)} \leq c\|\Delta \phi\|_{L_2(\Omega)}, \\
&\|\Delta u_f\|_{H^{1,0}(Q)} \leq c\|\Delta f h\|_{L_2(Q)} \leq c\|\Delta f\|_{L_2(\Omega)}\|h\|_{L_\infty(Q)},
\end{aligned}
$$

which conclude the proof of the first part at the lemma.

To prove the Fréchet differentiability in the q-component, consider the problem

$$\begin{cases} \frac{\partial v}{\partial t} = \nabla \cdot (k\nabla v) - qv - \Delta q u(q,\phi,f), & (x,t) \in Q, \\ k\frac{\partial v}{\partial \nu} + \alpha v = 0, \quad (x,t) \in S, \quad v(x,0) = 0, & x \in \overline{\Omega}, \end{cases} \tag{26}$$

where $\Delta q \in L_\infty(\Omega)$ such that $q + \Delta q \in \mathcal{A}_1$. Then, there exists a unique solution $v(x,t) \in H^{1,0}(Q)$ to the initial-boundary value problem (26), and the mapping $\Delta q \mapsto v$ from $L_\infty(\Omega)$ to $H^{1,0}(Q)$ defines a bounded linear operator $\mathcal{U}_q$ by the *a priori* estimate (6).

Denote $w := u(q + \Delta q, \phi, f) - u(q, \phi, f) - \mathcal{U}_q \Delta q = \Delta u_q - v$, where Δu_q satisfies the problem (23). Then, w satisfies the problem

$$\begin{cases} \frac{\partial w}{\partial t} = \nabla \cdot (k\nabla w) - qw - \Delta q \Delta u_q, & (x,t) \in Q, \\ k\frac{\partial w}{\partial \nu} + \alpha w = 0, \quad (x,t) \in S, \quad w(x,0) = 0, & x \in \overline{\Omega}. \end{cases}$$

By applying (6) and (20), we obtain

$$\|w\|_{H^{1,0}(Q)} \le c\|\Delta q \Delta u_q\|_{L_2(Q)} \le c\|\Delta q\|_{L_\infty(\Omega)}\|\Delta u_q\|_{L_2(Q)} \le c\|\Delta q\|_{L_\infty(\Omega)}\|\Delta u_q\|_{H^{1,0}(Q)} \le c\|\Delta q\|^2_{L_\infty(\Omega)}.$$

This implies that

$$\lim_{\|\Delta q\|_{L_\infty(\Omega)} \to 0} \frac{\|u(q + \Delta q, \phi, f) - u(q, \phi, f) - \mathcal{U}_q \Delta q\|_{H^{1,0}(Q)}}{\|\Delta q\|_{L_\infty(\Omega)}} = 0. \tag{27}$$

which means the differentiability in the q-component.

The differentiability in the ϕ and f components follows immediately from applying Theorem 1 and the estimate (6) to the initial boundary value problems (24) and (25), which imply that they have the unique solutions $\Delta u_\phi \in H^{1,0}(Q)$ and $\Delta u_f \in H^{1,0}(Q)$ and that the mappings $L_2(\Omega) \ni \Delta\phi \mapsto \Delta u_\phi \in H^{1,0}(Q)$ and $L_2(\Omega) \ni \Delta f \mapsto \Delta u_f \in H^{1,0}(Q)$ define the bounded linear operators $\mathcal{U}_\phi$ and $\mathcal{U}_f$, which, by definition, they satisfy $\mathcal{U}_\phi \Delta\phi = \Delta u_\phi = u(q, \phi + \Delta\phi, f) - u(q, \phi, f)$ and $\mathcal{U}_f \Delta f = \Delta u_f = u(q, \phi, f + \Delta f) - u(q, \phi, f)$, respectively. □

The CGM based on the gradient of $J(q, \phi, f)$ is applied to obtain the minimizer of the objective functional numerically. In order to obtain the gradient, we introduce the following adjoint problem:

$$\begin{cases} \frac{\partial \lambda}{\partial t} = -\nabla \cdot (k\nabla \lambda) + q\lambda - (u_1 - \phi_1^\epsilon)\delta(t - t_1) \\ \qquad -(u_2 - \phi_2^\epsilon)\delta(t - t_2) - 2(u_T - \phi_T^\epsilon)\delta(t - T), & (x,t) \in Q, \\ k\frac{\partial \lambda}{\partial \nu} + \alpha\lambda = 0, \quad (x,t) \in S, \quad \lambda(x,T) = 0, & x \in \overline{\Omega}, \end{cases} \tag{28}$$

where $\delta(\cdot)$ is the Dirac delta function. According to Definition 1, the weak solution $\lambda \in H^{1,0}(Q)$ of the adjoint problem (28), satisfies the variational equality

$$\begin{aligned} \int_Q \left(\lambda \frac{\partial \eta}{\partial t} + k\nabla\lambda \cdot \nabla\eta + q\lambda\eta \right) dxdt + \int_S \alpha\lambda\eta dsdt = \int_\Omega \{(u_1 - \phi_1^\epsilon)\eta(x, t_1) \\ +(u_2 - \phi_2^\epsilon)\eta(x, t_2) + (u_T - \phi_T^\epsilon)\eta(x, T)\} dx, \quad \forall \eta \in H^{1,1}(Q) \text{ with } \eta(\cdot, 0) = 0. \end{aligned} \tag{29}$$

Lemma 2. *Under the assumption of Theorem 1, there exists a constant $c > 0$, such that*

$$\|\lambda\|_{H^{1,0}(Q)} \le c(\|u_1 - \phi_1^\epsilon\|_{L_2(\Omega)} + \|u_2 - \phi_2^\epsilon\|_{L_2(\Omega)} + \|u_T - \phi_T^\epsilon\|_{L_2(\Omega)}) \le 3c\epsilon. \tag{30}$$

Proof. Multiplying by λ the first equation in (28) and integrating over Q using the boundary and initial conditions, we have

$$\frac{1}{2}\|\lambda(\cdot,0)\|^2_{L_2(\Omega)} + \int_Q \left\{k\nabla\lambda\cdot\nabla\lambda + q\lambda^2\right\} dxdt + \int_S \alpha\lambda^2 dsdt$$
$$= \int_\Omega \{(u_1-\phi_1^\epsilon)\lambda(x,t_1) + (u_2-\phi_2^\epsilon)\lambda(x,t_2) + (u_T-\phi_T^\epsilon)\lambda(x,T)\}\, dx.$$

Then, by (4), $q(x)\geq 0$ and $\alpha(x)\geq 0$, we have

$$\begin{aligned}
&\|\lambda\|^2_{H^{1,0}(Q)}\\
&\leq c(\|u_1-\phi_1^\epsilon\|_{L_2(\Omega)}\|\lambda(\cdot,t_1)\|_{L_2(\Omega)} + \|u_2-\phi_2^\epsilon\|_{L_2(\Omega)}\|\lambda(\cdot,t_2)\|_{L_2(\Omega)} + \|u_T-\phi_T^\epsilon\|_{L_2(\Omega)}\|\lambda(\cdot,T)\|_{L_2(\Omega)})\\
&\leq c(\|u_1-\phi_1^\epsilon\|_{L_2(\Omega)} + \|u_2-\phi_2^\epsilon\|_{L_2(\Omega)} + \|u_T-\phi_T^\epsilon\|_{L_2(\Omega)})\|\lambda\|_{H^{1,0}(Q)},
\end{aligned}$$

which means that the inequality (30) holds. □

Theorem 3. *The objective functional $J(q,\phi,f)$ is Fréchet differentiable, and the partial derivatives $J'_q(q,\phi,f)$, $J'_\phi(q,\phi,f)$, $J'_f(q,\phi,f)$ are given by*

$$J'_q(q,\phi,f) = -\int_0^T u(x,t)\lambda(x,t)dt, \tag{31}$$
$$J'_\phi(q,\phi,f) = \lambda(x,0), \tag{32}$$
$$J'_f(q,\phi,f) = \int_0^T \lambda(x,t)h(x,t)dt. \tag{33}$$

Proof. Taking $\Delta q\in L_\infty(\Omega)$ such that $q+\Delta q\in\mathcal{A}_1$, and denoting by $\Delta J_q = J(q+\Delta q,\phi,f) - J(q,\phi,f)$, the increment of the objective functional $J(q,\phi,f)$ in the q direction, then equation (18) yields

$$\Delta J_q = \int_\Omega \{\Delta u_{q,1}(u_1-\phi_1^\epsilon) + \Delta u_{q,2}(u_2-\phi_2^\epsilon) + \Delta u_{q,T}(u_T-\phi_T^\epsilon)\}\, dx$$
$$+\frac{1}{2}\left\{\|\Delta u_{q,1}\|^2_{L_2(\Omega)} + \|\Delta u_{q,2}\|^2_{L_2(\Omega)} + \|\Delta u_{q,T}\|^2_{L_2(\Omega)}\right\},$$

where $\Delta u_{q,1} := \Delta u_q(x,t_1;q,\phi,f)$, $\Delta u_{q,2} := \Delta u_q(x,t_2;q,\phi,f)$ and $\Delta u_{q,T} := \Delta u_q(x,T;q,\phi,f)$. Using the property of the Dirac delta function, the first term of the right hand side in the above formula can be written as

$$\int_\Omega \{\Delta u_{q,1}(u_1-\phi_1^\epsilon) + \Delta u_{q,2}(u_2-\phi_2^\epsilon) + \Delta u_{q,T}(u_T-\phi_T^\epsilon)\}\, dx$$
$$= \int_Q \Delta u_q \{(u_1-\phi_1^\epsilon)\delta(t-t_1) + (u_2-\phi_2^\epsilon)\delta(t-t_2) + 2(u_T-\phi_T^\epsilon)\delta(t-T)\}\, dxdt,$$

and by the adjoint problem (28), we have

$$\Delta J_q = \int_Q \Delta u_q \left\{-\frac{\partial\lambda}{\partial t} - \nabla\cdot(k\nabla\lambda) + q\lambda\right\} dx + \frac{1}{2}\left\{\|\Delta u_{q,1}\|^2_{L_2(\Omega)} + \|\Delta u_{q,2}\|^2_{L_2(\Omega)} + \|\Delta u_{q,T}\|^2_{L_2(\Omega)}\right\}.$$

Also, by (23) for Δu_q and integration by parts, we get

$$\int_Q \Delta u_q \left\{ -\frac{\partial \lambda}{\partial t} - \nabla \cdot (k \nabla \lambda) + q\lambda \right\} dxdt = -\int_\Omega \Delta u_q \lambda|_0^T dx$$
$$+ \int_Q \lambda \left\{ \frac{\partial (\Delta u_q)}{\partial t} - \nabla \cdot (k\nabla(\Delta u_q)) + q\Delta u_q \right\} dxdt + \int_S \left\{ k\frac{\partial(\Delta u_q)}{\partial \nu}\lambda - k\frac{\partial \lambda}{\partial \nu}\Delta u_q \right\} dsdt$$
$$= -\int_Q \Delta q u(q + \Delta q, \phi, f)\lambda dxdt = -\int_Q \Delta q \Delta u_q \lambda dxdt - \int_Q \Delta q u \lambda dxdt.$$

Thus, the above two equations and the property of the Dirac delta function imply

$$\Delta J_q = -\int_Q \Delta q \Delta u_q \lambda dxdt - \int_Q \Delta q u \lambda dxdt + \frac{1}{2}\left\{ \|\Delta u_{q,1}\|^2_{L_2(\Omega)} + \|\Delta u_{q,2}\|^2_{L_2(\Omega)} + \|\Delta u_{q,T}\|^2_{L_2(\Omega)} \right\}.$$

By the same approach for the problems (24) for Δu_ϕ and (25) for Δu_f, we can obtain

$$\Delta J_\phi = \int_\Omega \Delta\phi \lambda(x,0)dx + \frac{1}{2}\left\{ \|\Delta u_{\phi,1}\|^2_{L_2(\Omega)} + \|\Delta u_{\phi,2}\|^2_{L_2(\Omega)} + \|\Delta u_{\phi,T}\|^2_{L_2(\Omega)} \right\},$$
$$\Delta J_f = \int_Q \Delta f h \lambda dxdt + \frac{1}{2}\left\{ \|\Delta u_{f,1}\|^2_{L_2(\Omega)} + \|\Delta u_{f,2}\|^2_{L_2(\Omega)} + \|\Delta u_{f,T}\|^2_{L_2(\Omega)} \right\}.$$

From (6), we can obtain that

$$\max\{\|\Delta u_{q,1}\|^2_{L_2(\Omega)}, \|\Delta u_{q,2}\|^2_{L_2(\Omega)}, \|\Delta u_{q,T}\|^2_{L_2(\Omega)}\} \le \max_{t\in[0,T]} \|\Delta u_q(\cdot,t)\|^2_{L_2(\Omega)} \le c\|\Delta q\|^2_{L_\infty(\Omega)},$$
$$\max\{\|\Delta u_{\phi,1}\|^2_{L_2(\Omega)}, \|\Delta u_{\phi,2}\|^2_{L_2(\Omega)}, \|\Delta u_{\phi,T}\|^2_{L_2(\Omega)}\} \le \max_{t\in[0,T]} \|\Delta u_\phi(\cdot,t)\|^2_{L_2(\Omega)} \le c\|\Delta \phi\|^2_{L_2(\Omega)},$$
$$\max\{\|\Delta u_{f,1}\|^2_{L_2(\Omega)}, \|\Delta u_{f,2}\|^2_{L_2(\Omega)}, \|\Delta u_{f,T}\|^2_{L_2(\Omega)}\} \le \max_{t\in[0,T]} \|\Delta u_f(\cdot,t)\|^2_{L_2(\Omega)} \le c\|\Delta f\|^2_{L_2(\Omega)},$$

and via the estimate (30) and Lemma 1, we get

$$\left| \int_Q \Delta q \Delta u_q \lambda dxdt \right| \le \|\Delta q\|_{L_\infty(\Omega)} \|\lambda\|_{L_2(Q)} \|\Delta u_q\|_{L_2(Q)} \le c\|\Delta q\|^2_{L_\infty(\Omega)},$$

thus

$$\Delta J_q = -\int_Q \Delta q u \lambda dxdt + o(\|\Delta q\|_{L_\infty(\Omega)}), \quad \Delta J_\phi = \int_\Omega \Delta \phi \lambda(x,0)dx + o(\|\Delta\phi\|_{L_2(\Omega)}),$$
$$\Delta J_f = \int_Q \Delta f h \lambda dxdt + o(\|\Delta f\|_{L_2(\Omega)}), \tag{34}$$

which means that the formulae (31)–(33) for the Fréchet derivatives hold. The theorem is proved. □

4. Conjugate gradient method

In this section, the CGM will be developed and applied to obtain the numerical solutions for the reaction coefficient $q(x)$, the initial temperature $\phi(x)$ and the source term $f(x)$ to the inverse problem (2), (7)–(10). The following iterative process is used for the estimation of the triplet of functions (q, ϕ, f) by minimizing the objective functional (18):

$$q^{n+1} = q^n + \beta_q^n d_q^n, \quad \phi^{n+1} = \phi^n + \beta_\phi^n d_\phi^n, \quad f^{n+1} = f^n + \beta_f^n d_f^n, \quad n = 0, 1, 2, \cdots \tag{35}$$

with the search directions d_q^n, d_ϕ^n and d_f^n given by

$$d_q^n = \begin{cases} -J_q'^0, \\ -J_q'^n + \gamma_q^n d_q^{n-1}, \end{cases} \qquad d_\phi^n = \begin{cases} -J_\phi'^0, \\ -J_\phi'^n + \gamma_\phi^n d_\phi^{n-1}, \end{cases} \qquad d_f^n = \begin{cases} -J_f'^0, \\ -J_f'^n + \gamma_f^n d_f^{n-1}, \quad n = 1, 2, \cdots \end{cases} \tag{36}$$

where the subscript n indicates the number of iterations, q^0, ϕ^0 and f^0 are the initial guesses for the three unknown functions, $J_q'^n = J_q'(q^n, \phi^n, f^n)$, $J_\phi'^n = J_\phi'(q^n, \phi^n, f^n)$, $J_f'^n = J_f'(q^n, \phi^n, f^n)$, β_q^n, β_ϕ^n and β_f^n are the step sizes with respect to q, ϕ and f in passing from iteration n to the next iteration $n+1$. In our work, the Fletcher-Reeves formula [27] is applied for the conjugate gradient coefficients γ_q^n, γ_ϕ^n and γ_f^n given by

$$\gamma_q^n = \frac{\|J_q'^n\|^2_{L_2(\Omega)}}{\|J_q'^{n-1}\|^2_{L_2(\Omega)}}, \quad \gamma_\phi^n = \frac{\|J_\phi'^n\|^2_{L_2(\Omega)}}{\|J_\phi'^{n-1}\|^2_{L_2(\Omega)}}, \quad \gamma_f^n = \frac{\|J_f'^n\|^2_{L_2(\Omega)}}{\|J_f'^{n-1}\|^2_{L_2(\Omega)}}, \quad n = 1, 2, \cdots \tag{37}$$

Denote $u_1^n := u(x, t_1; q^n, \phi^n, f^n)$, $u_2^n := u(x, t_2; q^n, \phi^n, f^n)$ and $u_T^n := u(x, T; q^n, \phi^n, f^n)$, then the step sizes β_q^n, β_ϕ^n and β_f^n can be found by minimizing

$$J(q^{n+1}, \phi^{n+1}, f^{n+1}) = \frac{1}{2}\int_\Omega \left\{(u_1^{n+1} - \phi_1^\epsilon)^2 + (u_2^{n+1} - \phi_2^\epsilon)^2 + (u_T^{n+1} - \phi_T^\epsilon)^2\right\} dx.$$

Setting $\Delta q^n = d_q^n$, $\Delta\phi^n = d_\phi^n$ and $\Delta f^n = d_f^n$, the functions u_1^{n+1}, u_2^{n+1} and u_T^{n+1} are linearised by the Taylor series expansion in the following form:

$$\begin{aligned} & u(x, \bar t; q^n + \beta_q^n d_q^n, \phi^n + \beta_\phi^n d_\phi^n, f^n + \beta_f^n d_f^n) \approx u(x, \bar t; q^n, \phi^n, f^n) \\ & \quad + \beta_q^n d_q^n \frac{\partial u(x, \bar t; q^n, \phi^n, f^n)}{\partial q^n} + \beta_\phi^n d_\phi^n \frac{\partial u(x, \bar t; q^n, \phi^n, f^n)}{\partial \phi^n} + \beta_f^n d_f^n \frac{\partial u(x, \bar t; q^n, \phi^n, f^n)}{\partial f^n} \\ & \approx u(x, \bar t; q^n, \phi^n, f^n) + \beta_q^n \Delta u_q(x, \bar t; q^n, \phi^n, f^n) + \beta_\phi^n \Delta u_\phi(x, \bar t; q^n, \phi^n, f^n) + \beta_f^n \Delta u_f(x, \bar t; q^n, \phi^n, f^n) \end{aligned}$$

where $\bar t$ represents t_1, t_2 and T. Denote $\Delta u_{q,1}^n = \Delta u_q(x, t_1; q^n, \phi^n, f^n)$, $\Delta u_{q,2}^n = \Delta u_q(x, t_2; q^n, \phi^n, f^n)$ and $\Delta u_{q,T}^n = \Delta u_q(x, T; q^n, \phi^n, f^n)$, and $\Delta u_{\phi,1}^n$, $\Delta u_{\phi,2}^n$, $\Delta u_{\phi,T}^n$, $\Delta u_{f,1}^n$, $\Delta u_{f,2}^n$ and $\Delta u_{f,T}^n$ can be defined in the same way. We have

$$\begin{aligned} J(q^{n+1}, \phi^{n+1}, f^{n+1}) = & \frac{1}{2}\int_\Omega \left(u_1^n + \beta_q^n \Delta u_{q,1}^n + \beta_\phi^n \Delta u_{\phi,1}^n + \beta_f^n \Delta u_{f,1}^n - \phi_1^\epsilon\right)^2 dx \\ & + \frac{1}{2}\int_\Omega \left(u_2^n + \beta_q^n \Delta u_{q,2}^n + \beta_\phi^n \Delta u_{\phi,2}^n + \beta_f^n \Delta u_{f,2}^n - \phi_2^\epsilon\right)^2 dx \\ & + \frac{1}{2}\int_\Omega \left(u_T^n + \beta_q^n \Delta u_{q,T}^n + \beta_\phi^n \Delta u_{\phi,T}^n + \beta_f^n \Delta u_{f,T}^n - \phi_T^\epsilon\right)^2 dx. \end{aligned}$$

The partial derivatives of the objective functional $J(q^{n+1}, \phi^{n+1}, f^{n+1})$ with respect to β_q^n, β_ϕ^n and β_f^n are given by

$$\begin{aligned} & \frac{\partial J}{\partial \beta_q^n} = A_{11}\beta_q^n + A_{12}\beta_\phi^n + A_{13}\beta_f^n - B_1, \quad \frac{\partial J}{\partial \beta_\phi^n} = A_{21}\beta_q^n + A_{22}\beta_\phi^n + A_{23}\beta_f^n - B_2, \\ & \frac{\partial J}{\partial \beta_f^n} = A_{31}\beta_q^n + A_{32}\beta_\phi^n + A_{33}\beta_f^n - B_3, \end{aligned}$$

where $A_{12} = A_{21}$, $A_{13} = A_{31}$, $A_{23} = A_{32}$,

$$A_{11} = \sum_{i=1,2,T} \|\Delta u^n_{q,i}\|^2_{L_2(\Omega)}, \quad A_{22} = \sum_{i=1,2,T} \|\Delta u^n_{\phi,i}\|^2_{L_2(\Omega)}, \quad A_{33} = \sum_{i=1,2,T} \|\Delta u^n_{f,i}\|^2_{L_2(\Omega)},$$
$$A_{12} = \sum_{i=1,2,T} \langle \Delta u^n_{q,i}, \Delta u^n_{\phi,i}\rangle, \quad A_{13} = \sum_{i=1,2,T} \langle \Delta u^n_{q,i}, \Delta u^n_{f,i}\rangle, \quad A_{23} = \sum_{i=1,2,T} \langle \Delta u^n_{\phi,i}, \Delta u^n_{f,i}\rangle,$$

and

$$B_1 = -\sum_{i=1,2,T} \langle u^n_i - \phi^\epsilon_i, \Delta u^n_{q,i}\rangle, \quad B_2 = -\sum_{i=1,2,T} \langle u^n_i - \phi^\epsilon_i, \Delta u^n_{\phi,i}\rangle, \quad B_3 = -\sum_{i=1,2,T} \langle u^n_i - \phi^\epsilon_i, \Delta u^n_{f,i}\rangle.$$

Setting $\frac{\partial J}{\partial \beta^n_q} = \frac{\partial J}{\partial \beta^n_\phi} = \frac{\partial J}{\partial \beta^n_f} = 0$, the search step sizes β^n_q, β^n_ϕ and β^n_f can be obtained by solving the following linear system:

$$\mathcal{A}\mathbf{X} = \mathbf{B}, \tag{38}$$

where $\mathcal{A} = \{A_{ij}\}$, $i, j = \overline{1,3}$ is a symmetric matrix, $\mathbf{X} = \{\beta^n_q, \beta^n_\phi, \beta^n_f\}^{\mathrm{T}}$ and $\mathbf{B} = \{B_1, B_2, B_3\}^{\mathrm{T}}$.

The iteration process given by (35) does not provide the CGM with the stabilization necessary for the minimizing of the objective functional (18) to be classified as well-posed because of the errors inherent in the measured temperatures (8)–(10). However, the CGM may become well-posed if the discrepancy principle [11] is applied to stop the iteration procedure at the smallest threshold n for which

$$J(q^n, \phi^n, f^n) \approx \bar{\epsilon}, \tag{39}$$

where $\bar{\epsilon}$ is a small positive value, e.g., $\bar{\epsilon} = 10^{-5}$ for exact temperature measurements, and

$$\bar{\epsilon} = \frac{1}{2}\left(\|\phi^\epsilon_1 - \phi_1\|^2_{L_2(\Omega)} + \|\phi^\epsilon_2 - \phi_2\|^2_{L_2(\Omega)} + \|\phi^\epsilon_T - \phi_T\|^2_{L_2(\Omega)}\right), \tag{40}$$

if the measured temperatures contain noise. Based on (11), we indicate that $\bar{\epsilon} \leq 3\epsilon^2/2$.

In summary, the CGM for the numerical estimation of the space-dependent reaction coefficient $q(x)$, initial temperature $\phi(x)$ and source term $f(x)$ is presented as follows:

S1. Set $n = 0$ and choose initial guesses q^0, ϕ^0 and f^0 for the three unknown coefficients $q(x)$, $\phi(x)$ and $f(x)$, respectively.

S2. Solve the initial-boundary value direct problem (2), (3) and (7) numerically by using the FDM to compute $u(x, t; q^n, \phi^n, f^n)$, and $J(q^n, \phi^n, f^n)$ by (18).

S3. Solve the adjoint problem (28) to obtain $\lambda(x, t; q^n, \phi^n, f^n)$, and the Fréchet gradients J'^n_q in (31), J'^n_ϕ in (32) and J'^n_f in (33). Compute the conjugate coefficients γ^n_q, γ^n_ϕ and γ^n_f in (37), and the search directions d^n_q, d^n_ϕ and d^n_f in (36).

S4. Solve the sensitivity problems (23) for $\Delta u_q(x, t; q^n, \phi^n, f^n)$, (24) for $\Delta u_\phi(x, t; q^n, \phi^n, f^n)$, and (25) for $\Delta u_f(x, t; q^n, \phi^n, f^n)$ by taking $\Delta q^n = d^n_q$, $\Delta\phi^n = d^n_\phi$ and $\Delta f^n = d^n_f$, and compute the search step sizes β^n_q, β^n_ϕ and β^n_f by (38).

S5. Update q^{n+1}, ϕ^{n+1} and f^{n+1} by (35).

S6. If the stopping criterion (39) is satisfied, then go to S7. Else set $n = n + 1$, and go to S2.

S7. End.

5. Numerical results and discussion

In this section, the space-dependent reaction coefficient $q(x)$, the initial temperature $\phi(x)$ and the source term $f(x)$ are simultaneously reconstructed by the CGM proposed in Section 4. The FDM based on the Crank-Nicolson scheme [28] is applied to solve the direct, sensitivity and adjoint problem involved. Note that in the adjoint problem (28), we approximate the Dirac delta function $\delta(\cdot)$ by

$$\delta_a(t-\tilde{t}) = \frac{1}{a\sqrt{\pi}} e^{-(t-\tilde{t})^2/a^2}, \tag{41}$$

where a is a small positive constant taken as, e.g., $a = 10^{-3}$, and $\tilde{t}$ represents t_1, t_2 and T. The accuracy errors, as functions of the iteration numbers n, for $q(x)$, $\phi(x)$ and $f(x)$ are defined as

$$E_1(q^n) = \|q^n - q\|_{L_2(\Omega)}, \tag{42}$$
$$E_2(\phi^n) = \|\phi^n - \phi\|_{L_2(\Omega)}, \tag{43}$$
$$E_3(f^n) = \|f^n - f\|_{L_2(\Omega)}, \tag{44}$$

where q^n, ϕ^n and f^n are the numerical solutions obtained by the CGM at the iteration number n, and q, ϕ and f are the analytical expressions for the reaction coefficient, initial temperature and source term, if available.

The measured noisy temperatures ϕ_1^ϵ, ϕ_2^ϵ and ϕ_T^ϵ are simulated by adding the Gaussian noisy term to the true temperatures

$$\phi_i^\epsilon = \phi_i + \sigma \times \text{random}(1), \quad i = 1, 2, T, \tag{45}$$

where $\sigma = \frac{p}{100} \max_{x\in\overline{\Omega}} \{|\phi_1(x)|, |\phi_2(x)|, |\phi_T(x)|\}$ is the standard deviation, $p\%$ represents the percentage of noise, and random(1) generates random values from a normal distribution with zero mean and unit standard deviation.

We consider a couple of one-dimensional ($N = 1$) test examples in a finite slab $\Omega = (0, 1)$ over the time period $T = 1$. For the numerical discretisation we employ the FDM with a mesh of 100 equidistant nodes equally spread over each of the space and time intervals.

5.1. Example 1

In this example, we take $t_1 = 0.5$, $t_2 = 0.7$ and

$$\begin{aligned}
&k \equiv 1, \quad \alpha \equiv 1, \quad g(x,t) = x(1+x)^2 e^{-t} - (1+x)(1+x^3)t^3, \\
&h(x,t) = (1+x)t^3, \quad \mu(0,t) = e^{-t}, \quad \mu(1,t) = 4e^{-t}, \\
&\phi_1(x) = e^{-0.5}(1+x^2), \quad \phi_2(x) = e^{-0.7}(1+x^2), \quad \phi_T(x) = e^{-1}(1+x^2).
\end{aligned}$$

Based on this input data, the analytical solution to the inverse problem (2), (7)–(10) is given by

$$q(x) = 3 + x, \quad \phi(x) = 1 + x^2, \quad f(x) = 1 + x^3, \quad u(x,t) = (1+x^2)e^{-t}. \tag{46}$$

The initial guesses are chosen as $q^0(x) = 2$, $\phi^0(x) = 2 + x$ and $f^0(x) = 1$. Figure 1(a) shows the objective functional $J(q^n, \phi^n, f^n)$ given by (18) for the simultaneous reconstruction of the three unknown coefficients with $p \in \{0, 1\}$ noise. From this figure it can be seen that the objective functional (18), as a function of iteration numbers n, is rapidly monotonic decreasing convergent. The stopping iteration number is 30 for exact data, i.e., $p = 0$, whilst the algorithm is stopped at the iteration number 4 for $p = 1$ noise, obtained according to the discrepancy principle (39). The accuracy errors $E_1(q^n)$ given by (42), $E_2(\phi^n)$ given by (43) and $E_3(f^n)$ given by (44) are shown in Figures 1(b)–1(d), respectively. From these figures, it can be seen that for $p = 0$, the accuracy errors keep decreasing as the iterations proceed, but for $p = 1$ noise the errors start quickly increasing after just a few iterations. Therefore, stopping the CGM iterations after 4 iterations, (cf. Figure 1(a)), will yield stable and reasonably accurate numerical solutions, as illustrated in Figure 2. The larger errors near the boundary endpoints $x = 0$ and $x = 1$ are somewhat expected because the initial guesses are quite far from their exact values near these points. In such situations, the use of the preconditioner Sobolev gradients [29] instead of the L_2-gradients (31)–(33) may improve the accuracy of the numerical reconstructions near the boundary $\partial\Omega$.

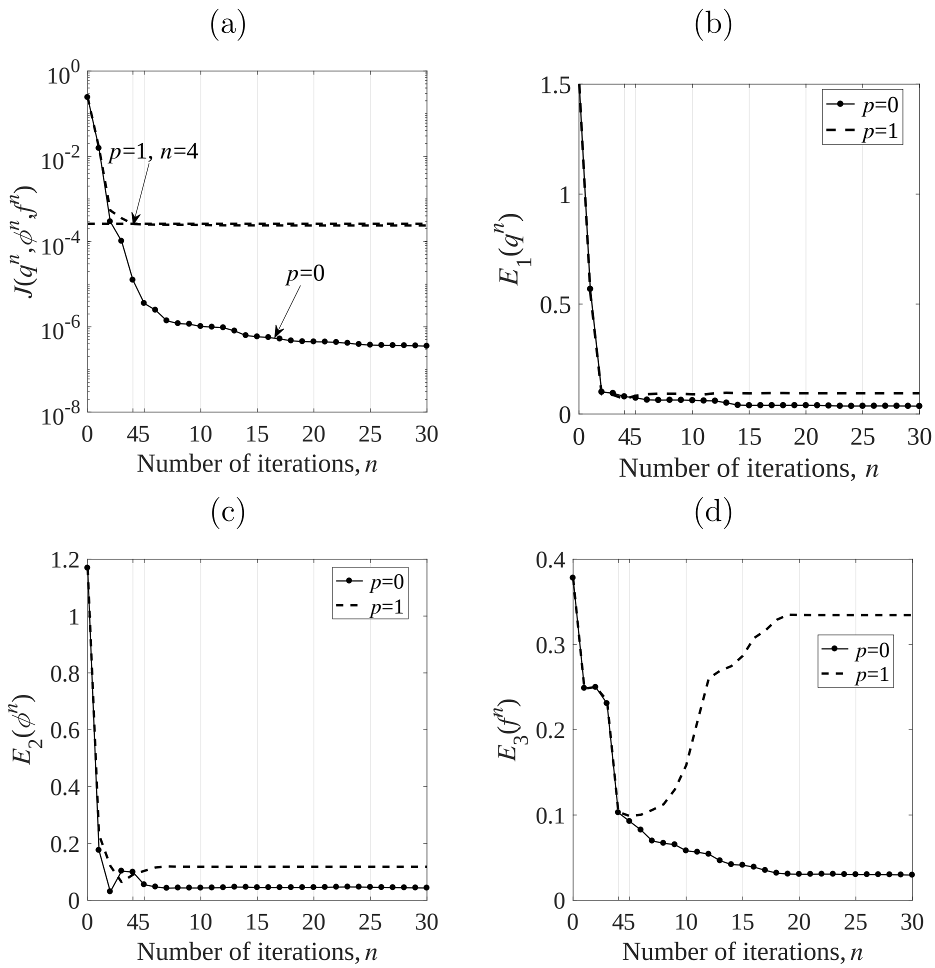

Figure 1: (a) The objective functional (18) and the accuracy errors (b) (42) (c) (43) and (d) (44), with $p \in \{0, 1\}$ noise, for Example 1.

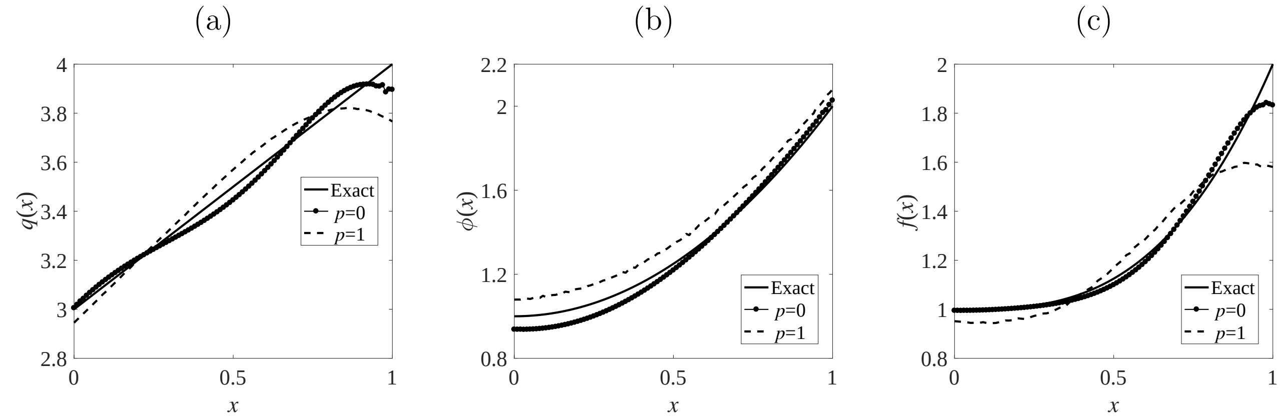

Figure 2: The exact and numerical solutions for (a) the reaction coefficient $q(x)$, (b) the initial temperature $\phi(x)$ and (c) the source term $f(x)$, with $p \in \{0, 1\}$ noise, for Example 1.

5.2. Example 2

We take $t_1 = 0.3$, $t_2 = 0.7$ and

$$k \equiv 1, \quad \alpha \equiv 1, \quad h(x,t) = (2 + x^3)e^t, \quad \mu(0,t) = \mu(1,t) = e^{-t},$$

$$g(x,t) = \pi^2 \sin(\pi x)e^{-t} - (3 - 2x^2)(2 + x^3)e^t + (1 + \pi + \sin(\pi x))e^{-t} \begin{cases} 1 - x, & x \in [0, 0.3], \\ -x + 4x^2, & x \in (0.3, 0.7), \\ 2 & x \in [0.7, 1], \end{cases}$$

$$\phi_1(x) = e^{-0.3}(1 + \pi + \sin(\pi x)), \quad \phi_2(x) = e^{-0.7}(1 + \pi + \sin(\pi x)),$$
$$\phi_T(x) = e^{-1}(1 + \pi + \sin(\pi x)).$$

Based on this input data, the analytical solution to the inverse problem (2), (7)–(10) is given by

$$q(x) = \begin{cases} 2 - x, & x \in [0, 0.3], \\ 1 - x + 4x^2, & x \in (0.3, 0.7), \\ 3, & x \in [0.7, 1], \end{cases} \qquad f(x) = 3 - 2x^2,$$
$$\phi(x) = 1 + \pi + \sin(\pi x), \quad u(x,t) = (1 + \pi + \sin(\pi x))e^{-t}. \tag{47}$$

In comparison with the Example 1, this example is more severe since the reaction coefficient $q(x)$ in (47) to be retrieved is a discontinuous function. The initial guesses are taken as $q^0(x) = 1$, $\phi^0(x) = 1$ and $f^0(x) = 1$. Figure 3(a) shows the convergence of the objective functional $J(q^n, \phi^n, f^n)$ given by (18) with the iterative CGM stopped at the iteration numbers $\{50, 18\}$ for $p \in \{0, 1\}$ noise, respectively. The corresponding numerical solutions to the reaction coefficient $q(x)$, the initial temperature $\phi(x)$ and the source term $f(x)$ at these stopping iteration numbers are illustrated in Figures 3(b)–3(d), respectively. From these figures, it can be seen that the retrieved results are reasonably accurate and stable bearing in mind the severe discontinuous reaction coefficient that had to be recovered along with the initial temperature and the source term, simultaneously.

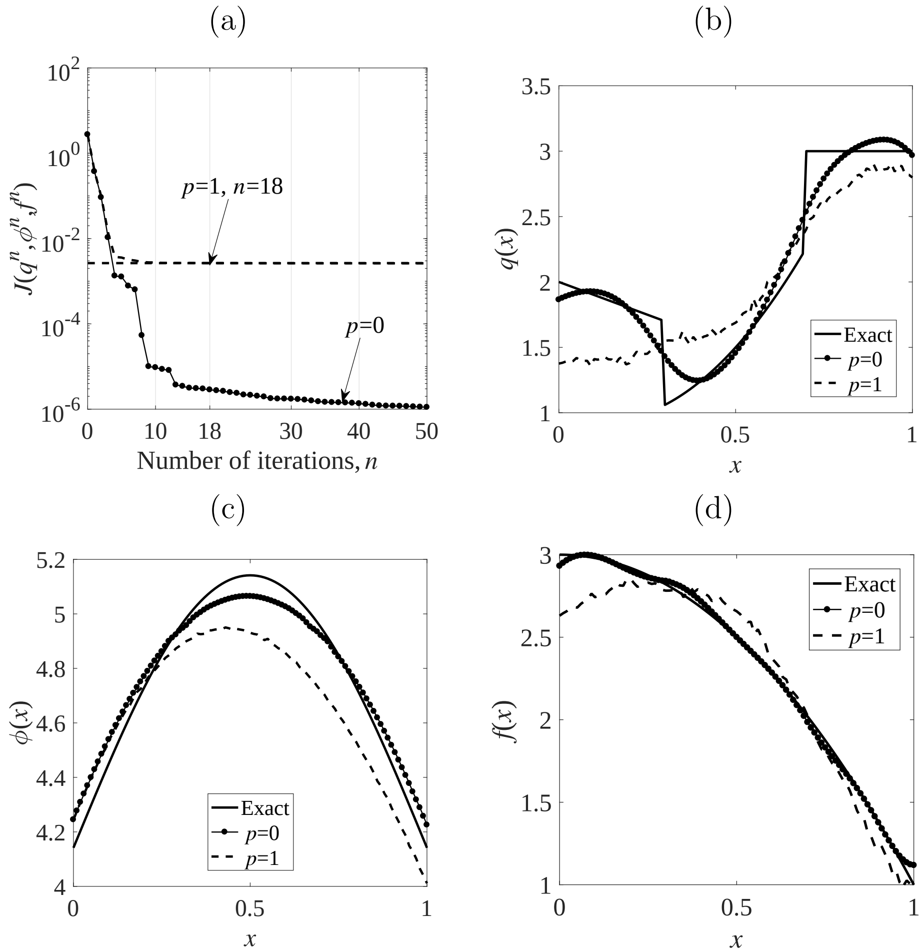

Figure 3: (a) The objective functional (18) and the exact and numerical solutions for (b) the reaction coefficient $q(x)$, (c) the initial temperature $\phi(x)$ and (d) the source term $f(x)$, with $p \in \{0, 1\}$ noise, for Example 2.

6. Conclusions

The simultaneous retrieval of the space-dependent reaction coefficient, the initial temperature and the source term from the measured temperatures at two time instants t_1, t_2 and at the final time T has been investigated. The three unknown coefficients have been reconstructed by minimizing the least-squares objective functional. Based on a variational method, the Fréchet derivatives with respect to the three unknowns are obtained together with the adjoint and sensitivity problems. The CGM has then been applied to numerically retrieve the three unknown coefficients. Two numerical examples for one-dimensional inverse problems have been illustrated for continuous and discontinuous reaction coefficient. The numerical solutions regularized by the discrepancy principle have been obtained accurate and stable for all the three space-dependent unknown quantities that have been simultaneously retrieved. Immediate beneficiaries of this research would be the engineering heat transfer community concerned with practical situations involving unknown reaction coefficients, heat sources and the initial temperature status. Also, in order to increase the impact of the performed research, future work will be concerned with inverting real raw temperature data obtained from a finned tube heat exchanger.

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References

[1] K. Kurpisz, A. J. Nowak, Inverse Thermal Problems, Computational Mechanics Publications Southampton, 1995.

[2] W. Rundell, The determination of a parabolic equation from initial and final data, Proceedings of the American Mathematical Society 99 (4) (1987) 637–642.

[3] A. I. Prilepko, V. V. Solov'ev, Solvability of the inverse boundary-value problem of finding a coefficient of a lower-order derivative in a parabolic equation, Differential Equations 23 (1) (1987) 101–107.

[4] V. Isakov, Inverse parabolic problems with the final overdetermination, Communications on Pure and Applied Mathematics 44 (2) (1991) 185–209.

[5] A. I. Prilepko, A. B. Kostin, On certain inverse problems for parabolic equations with final and integral observation, Russian Academy of Science Siberian Mathematics 75 (1993) 473–490.

[6] Q. Chen, J. Liu, Solving an inverse parabolic problem by optimization from final measurement data, Journal of Computational and Applied Mathematics 193 (1) (2006) 183–203.

[7] K. Cao, D. Lesnic, Reconstruction of the space-dependent perfusion coefficient from final time or time-average temperature measurements, Journal of Computational and Applied Mathematics 337 (2018) 150–165.

[8] V. Isakov, Inverse Source Problems, American Mathematical Society, 1990.

[9] V. Isakov, Inverse Problems for Partial Differential Equation, Springer-Verlag, 2006.

[10] A. I. Prilepko, D. G. Orlovsky, I. A. Vasin, Methods for Solving Inverse Problems in Mathematical Physics, CRC Press, New York, 2000.

[11] O. M. Alifanov, Inverse Heat Transfer Problems, Springer Science & Business Media, Berlin, 2012.

[12] M. N. Ozisik, H. R. B. Orlande, Inverse Heat Transfer: Fundamentals and Applications, CRC Press, Taylor & Francis, New York, 2000.

[13] H. Han, D. Ingham, Y. Yuan, The boundary element method for the solution of the backward heat conduction equation, Journal of Computational Physics 116 (2) (1995) 292–299.

[14] D. Lesnic, L. Elliott, D. Ingham, An iterative boundary element method for solving the backward heat conduction problem using an elliptic approximation, Inverse Problems in Engineering 6 (4) (1998) 255–279.

[15] C.-L. Fu, X.-T. Xiong, Z. Qian, Fourier regularization for a backward heat equation, Journal of Mathematical Analysis and Applications 331 (1) (2007) 472–480.

[16] C.-S. Liu, A self-adaptive LGSM to recover initial condition or heat source of one-dimensional heat conduction equation by using only minimal boundary thermal data, International Journal of Heat and Mass Transfer 54 (7) (2011) 1305–1312.

[17] M. Yamamoto, J. Zou, Simultaneous reconstruction of the initial temperature and heat radiative coefficient, Inverse Problems 17 (4) (2001) 1181–1202.

[18] M. Choulli, M. Yamamoto, Uniqueness and stability in determining the heat radiative coefficient, the initial temperature and a boundary coefficient in a parabolic equation, Nonlinear Analysis: Theory, Methods & Applications 69 (11) (2008) 3983–3998.

[19] B. T. Johansson, D. Lesnic, A procedure for determining a spacewise dependent heat source and the initial temperature, Applicable Analysis 87 (3) (2008) 265–276.

[20] H. W. Engl, M. Hanke, A. Neubauer, Regularization of Inverse Problems, Vol. 375, Springer Science & Business Media, Berlin, 1996.

[21] F. Tröltzsch, Optimal Control of Partial Differential Equations: Theory, Methods, and Applications, Vol. 112, American Mathematical Society, 2010.

[22] K. Cao, D. Lesnic, Simultaneous reconstruction of the perfusion coefficient and initial temperature from time-average integral temperature measurements, Applied Mathematical Modelling 68 (2019) 523–539.

[23] J. R. Cannon, H. M. Yin, A class of non-linear non-classical parabolic equations, Journal of Differential Equations 79 (2) (1989) 266–288.

[24] J. R. Cannon, M. Salman, On a class of nonlinear nonclassical parabolic equations, Applicable Analysis 85 (1-3) (2006) 23–44.

[25] Y. L. Keung, J. Zou, Numerical identifications of parameters in parabolic systems, Inverse Problems 14 (1) (1998) 83–100.

[26] D. N. Hào, P. X. Thanh, D. Lesnic, Determination of the heat transfer coefficients in transient heat conduction, Inverse Problems 29 (2013) 095020 (21 pp).

[27] R. Fletcher, C. M. Reeves, Function minimization by conjugate gradients, The Computer Journal 7 (2) (1964) 149–154.

[28] R. D. Richtmyer, K. W. Morton, Difference Methods for Initial-Value Problems, Interscience Publishers John Wiley & Sons, Inc., New York, 1967.

[29] B. Jin, J. Zou, Numerical estimation of the Robin coefficient in a stationary diffusion equation, IMA Journal of Numerical Analysis 30 (3) (2010) 677–701.