Determination of time-dependent coefficients in moving boundary problems under nonlocal and heat moment observations

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Abstract
This paper investigates the reconstruction of time-dependent coefficients in the transient heat equation in a moving boundary domain with unknown free boundaries. This problem is considered under Stefan/heat moments overdetermination conditions also dependent of time. This inverse problem is nonlinear. Moreover, although local existence and uniqueness of solution hold, the problem is still ill-posed since small errors into the input data lead to large errors in the reconstructed coefficients. In order to obtain a stable solution, the nonlinear Tikhonov regularization method is employed. This recasts as minimizing a regularization functional subject to simple bounds on variables. Numerically, this is accomplished using the Matlab toolbox optimization routine *lsqnonlin*. Numerical results illustrate that stable and accurate solutions are obtained.

Keywords: Moving boundary problem; inverse problem; coefficient identification problem; nonlinear optimization, reaction-diffusion equation.

1 Introduction

Inverse geometry problems, e.g. inverse Stefan problems, arise in many technological processes related to phase change [5]. In [4, 7, 9], the authors produced numerical solutions to various moving boundary inverse problems under Stefan/heat moments overdetermination conditions. In [12], the author investigated the unique solvability of inverse coefficient identification problems with free boundaries (two-sided Stefan problem). In the present paper, we advance on these related studies and investigate the possibility of reconstructing numerically both moving boundaries of a one-dimensional finite slab along with the time-dependent raection coefficient from initial and boundary conditions, supplemented by nonlocal and integral observations that may contain errors.

The organization of this paper is as follows. Section 2 presents the mathematical formulation of the inverse problem with Stefan condition as overspeciefied data, while Section 3 presents another formulation of the problem with heat moments. The numerical procedure for solving inverse problems is described in Section 4 and the obtained results are presented and discussed in Section 5. Finally, conclusions are highlighted in Section 6.

2 Statements of the inverse problems

In the moving domain $\Omega_T := \{(x,t) : h_1(t) < x < h_2(t),\ 0 < t < T\}$, where $h_1(t) < h_2(t)$, we consider the inverse problem consisting in the determination of the free boundaries $h_1(t)$ and $h_2(t)$, along with the temperature $u(x,t)$ and the intensity of reaction (or heat transfer, perfusion or radiative) coefficient $c(t)$ satifying the one-dimensional time-dependent parabolic equation

$$u_t = a(x,t)u_{xx} + b(x,t)u_x + c(t)u + f(x,t), \quad (x,t) \in \Omega_T, \tag{1}$$

where $a > 0$ and b are a given functions and f is a given heat source, subject to the initial condition

$$u(x,0) = \phi(x), \quad x \in [h_1(0), h_2(0)], \tag{2}$$

where $h_1(0) = h_{01}$ and $h_2(0) = h_{02}$ are given numbers satisfying $h_{01} < h_{02}$, the Dirichlet boundary conditions

$$u(h_1(t),t) = \mu_1(t), \quad u(h_2(t),t) = \mu_2(t), \quad t \in [0,T], \tag{3}$$

and the over-determination conditions

$$h_1'(t) - u_x(h_1(t),t) = \mu_3(t), \quad t \in [0,T], \tag{4}$$

$$h_2'(t) + u_x(h_2(t),t) = \mu_4(t), \quad t \in [0,T], \tag{5}$$

$$\int_{h_1(t)}^{h_2(t)} u(x,t)dx = \mu_5(t), \quad t \in [0,T], \tag{6}$$

where $\phi(x)$ and $\mu_i(t)$ for $i = \overline{1,5}$ are given functions satisfying the compatibility conditions

$$\phi(h_{01}) = \mu_1(0), \quad \phi(h_{02}) = \mu_2(0). \tag{7}$$

Note that the equations (4) and (5) represent Stefan conditions of melting between a solid and liquid. Also, equation (6) represents the mass (energy) specification [2]. The leading part of the right-hand side of equation (1) could be written in the usual divergence form by remarking that $a(x,t)u_{xx} + b(x,t)u_x = (a(x,t)u_x)_x + (b(x,t) - a_x(x,t))u_x$.

The inverse problem is concerned with the invertibility of the map $(\mu_3, \mu_4, \mu_5) \mapsto (h_1(t), h_2(t), c(t))$. Introducing the Landau's transformation $y = (x - h_1(t))/(h_2(t) - h_1(t))$, we recast the problem (1)-(6) into the following inverse problem for the unknowns $(h_1(t), h_3(t), c(t), v(y,t))$, where $h_3(t) := h_2(t) - h_1(t)$ and $v(yh_3(t) + h_1(t), t) = u(x,t)$, [12]:

$$v_t = \frac{a(yh_3(t) + h_1(t), t)}{h_3^2(t)} v_{yy} + \frac{b(yh_3(t) + h_1(t), t) + yh_3'(t) + h_1'(t)}{h_3(t)} v_y$$
$$+ c(t)v + f(yh_3(t) + h_1(t), t), \quad (y,t) \in Q_T, \tag{8}$$

in the fixed domain $Q_T := \{(y,t) : 0 < y < 1, 0 < t < T\} = (0,1) \times (0,T)$,

$$v(y,0) = \phi(yh_3(0) + h_1(0)), \quad y \in [0,1], \tag{9}$$

$$v(0,t) = \mu_1(t), \quad v(1,t) = \mu_2(t), \quad t \in [0,t], \tag{10}$$

$$h_1'(t) - \frac{v_y(0,t)}{h_3(t)} = \mu_3(t), \quad t \in [0,T], \tag{11}$$

$$h_3'(t) + \frac{v_y(0,t) + v_y(1,t)}{h_3(t)} + \mu_3(t) = \mu_4(t), \quad t \in [0,T], \tag{12}$$

$$h_3(t) \int_0^1 v(y,t)dy = \mu_5(t), \quad t \in [0,T], \tag{13}$$

Definition 1. *As a solution of the inverse problem (8)–(13), we define the quadruplet* $(h_1(t), h_3(t), c(t), v(y,t)) \in ((C^1[0,T])^2 \times C[0,T] \times (C^{2,1}(Q_T) \cap C^{1,0}(\overline{Q}_T)))$, $h_3(t) > 0$ *for* $t \in [0,T]$, *that satisfies equations (8)–(13).*

The local existence and uniqueness of the solution of problem (8)–(13) (and, via the transformations $h_2(t) = h_1(t) + h_3(t)$ and $u(x,t) = v(yh_3(t) + h_1(t), t)$, also of the problem (1)-(6)) were established in [12], and read as follows.

Theorem 1 (local existence of solution)**.** *Assume that the following conditions are satisfied:*

1. $b, f \in C^{1,0}(\mathbb{R} \times [0,T])$, $\phi \in C^1[h_{01}, \infty)$, $\mu_i \in C^1[0,T]$, $i = 1,2,3$;
2. $a \in C^{1,0}(\mathbb{R} \times [0,T])$, $a_x(x,t)$ *is Holder continuous with exponent* $\alpha \in (0,1)$, *and* $\mu_j \in C[0,T]$, $j = 3,4$;
3. $0 < a_0 \le a(x,t) \le a_1$, $|a_x(x,t)| \le a_2$, $|b(x,t)| \le b_0$, $0 < f(x,t) \le f_0$, $|f_x(x,t)| \le f_1$ *for* $(x,t) \in \mathbb{R} \times [0,T]$, $0 < \phi_0 \le \phi(x) \le \phi_1$ *for* $x \in [h_{01}, \infty)$, $\mu_i(t) > 0$, $i = 1,2,3$, *for* $t \in [0,T]$; *where* a_0, a_1, a_2, b_0, f_0, f_1, ϕ_0 *and* ϕ_1 *are given positive constants.*
4. *The compatibility conditions (7).*

Then, it is possible to specify a time $T_0 \in (0,T]$, *which is determined by the input data, such that there exists a (local) solution to the inverse problem (8)-(13) for* $(y,t) \in Q_{T_0}$.

The initial value of $c(0)$ can be calculated as follows. Using Leibniz's rule for differentiation under the integral sign, differentiate equation (6) to obtain

$$\frac{d}{dt}\left(\int_{h_1(t)}^{h_2(t)} u(x,t)dx\right) = u(h_2(t),t)h_2'(t) - u(h_1(t),t)h_1'(t) + \int_{h_1(t)}^{h_2(t)} u_t(x,t)dx$$
$$= \mu_2(t)h_2'(t) - \mu_1(t)h_1'(t) + \int_{h_1(t)}^{h_2(t)} u_t(x,t)dx = \mu_5'(t), \quad t \in [0,T]. \tag{14}$$

By using the overdetermination conditions (4) and (5), equation (14) becomes

$$\int_{h_1(t)}^{h_2(t)} u_t(x,t)dx = \mu_5'(t) + \mu_1(t)u_x(h_1(t),t) + \mu_1(t)\mu_3(t) + \mu_2(t)u_x(h_2(t),t) - \mu_2(t)\mu_4(t). \tag{15}$$

On the other hand, integrating equation (1) with respect to x over the interval $[h_1(t), h_2(t)]$, we obtain

$$\int_{h_1(t)}^{h_2(t)} u_t(x,t)dx = \int_{h_1(t)}^{h_2(t)} [a(x,t)u_{xx}(x,t) + b(x,t)u_x(x,t) + f(x,t)]\,dx + c(t)\mu_5(t). \quad (16)$$

By equating (15) and (16) we obtain

$$\int_{h_1(t)}^{h_2(t)} [a(x,t)u_{xx}(x,t) + b(x,t)u_x(x,t) + f(x,t)]\,dx + c(t)\mu_5(t)$$
$$= \mu_5'(t) + \mu_1(t)u_x(h_1(t),t) + \mu_1(t)\mu_3(t) + \mu_2(t)u_x(h_2(t),t) - \mu_2(t)\mu_4(t),$$

from which

$$c(t) = \frac{1}{\mu_5(t)}\Big[\mu_5'(t) + \mu_1(t)u_x(h_1(t),t) + \mu_1(t)\mu_3(t) + \mu_2(t)u_x(h_2(t),t) - \mu_2(t)\mu_4(t)$$
$$- \int_{h_1(t)}^{h_2(t)} [a(x,t)u_{xx}(x,t) + b(x,t)u_x(x,t) + f(x,t)]\,dx\Big].$$

Now evaluating the last equation at the initial time $t = 0$, we obtain

$$c(0) = \frac{1}{\mu_5(0)}\Big[\mu_5'(0) + \mu_1(0)\phi'(h_{01}) + \mu_1(0)\mu_3(0) + \mu_2(0)\phi'(h_{02}) - \mu_2(0)\mu_4(0)$$
$$- \int_{h_{01}}^{h_{20}} [a(x,0)\phi''(x) + b(x,0)\phi'(x) + f(x,0)]\,dx\Big], \quad (17)$$

where all the quantities are known. The values of $h_1'(0)$ and $h_2'(0)$ can also be obtained from the compatibility between (2), (4) and (5), as given by:

$$h_1'(0) = \mu_3(0) + \phi'(h_{01}), \quad h_2'(0) = \mu_4(0) - \phi'(h_{02}). \quad (18)$$

Theorem 2 (uniqueness of the solution)**.** *Assume that the following conditions are satisfied:*

1. $a \in C^{2,0}(\mathbb{R} \times [0,T])$, b, $f \in C^{1,0}(\mathbb{R} \times [0,T])$
2. $a(x,t) > 0$ *for* $(x,t) \in \mathbb{R} \times [0,T]$
3. $\phi(x) \geq \phi_0 > 0$ *for* $x \in [h_{01}, \infty)$
4. $\mu_5(t) > 0$ *for* $t \in [0,T]$.

Then, the inverse problem (8)–(13) cannot have more than one solution.

3 Another related inverse problem formulation

It was pointed out in [12] that the Stefan conditions (4) and (5) or, (11) and (12), can be replaced by the heat moments of first- and second-order

$$\int_{h_1(t)}^{h_2(t)} xu(x,t)dx = \mu_6(t), \quad t \in [0,T], \quad (19)$$

$$\int_{h_1(t)}^{h_2(t)} x^2u(x,t)dx = \mu_7(t), \quad t \in [0,T], \quad (20)$$

or, in terms of transformation $y = \frac{x-h_1(t)}{h_2(t)-h_1(t)}$, by

$$h_3^2(t)\int_0^1 yv(y,t)dy + h_1(t)\mu_5(t) = \mu_6(t), \quad t \in [0,T], \tag{21}$$

$$h_3^3(t)\int_0^1 y^2v(y,t)dy - h_1^2(t)\mu_5(t) + 2h_1(t)\mu_6(t) = \mu_7(t), \quad t \in [0,T]. \tag{22}$$

respectively. Definition 1 is still valid for the solution of the inverse problem (8)-(10), (13), (21), (22), which is concerned with the possible invertibility of the map $(\mu_5, \mu_6, \mu_7) \mapsto (h_1, h_2, c)$. The local existence and global uniqueness of solution to this problem were established in [12], and are stated as follows.

Theorem 3 (local existence of solution)**.** *Assume that the following conditions are satisfied:*

1. *$b, f \in C^{1,0}(\mathbb{R} \times [0,T])$, $\phi \in C^1[h_{01}, \infty)$, $\mu_i \in C^1[0,T]$, $i = 1, 2, 5$;*
2. *$a \in C^{2,0}(\mathbb{R} \times [0,T])$, $\mu_j \in C^1[0,T]$, $j = 6, 7$;*
3. *$0 < a_0 \leq a(x,t) \leq a_1$, $|a_x(x,t)| \leq a_2$, $|b(x,t)| \leq b_0$, $0 < f(x,t) \leq f_0$, $|f_x(x,t)| \leq f_1$ for $(x,t) \in \mathbb{R} \times [0,T]$, where a_0, a_1, a_2, b_0, f_0 and f_1 are given constants. Also, $0 < \phi_0 \leq \phi(x) \leq \phi_1$ for $x \in [h_{01}, \infty)$, $\mu_i(t) > 0$, $i = 1, 2, 5$, for $t \in [0,T]$.*
4. *The compatibility conditions (7) and*

$$\int_{h_{01}}^{h_{02}} x\phi(x)dx = \mu_6(0), \quad \int_{h_{01}}^{h_{02}} x^2\phi(x)dx = \mu_7(0). \tag{23}$$

Then, we can specify a time $T_1 \in (0,T]$, which can be determined by the input data, such that there exists a (local) solution to the inverse problem (8)-(10), (13), (21)-(22) for $(y,t) \in Q_{T_1}$.

Theorem 4 (uniqueness of the solution)**.** *Assume that the conditions of Theorem 2 hold. Then, the inverse problem (8)-(10), (13), (21)-(22) cannot have more than one solution.*

As in the previous inverse problem, we can also find the value of $c(0)$, $h_1'(0)$ and $h_2'(0)$, as follows. Differentiating equations (6), (19) and (20) we obtain:

$$\mu_5'(t) - \int_{h_1(t)}^{h_2(t)} [a(x,t)u_{xx} + b(x,t)u_x + f(x,t)]dx = \mu_2(t)h_2'(t) - \mu_1(t)h_1'(t) + c(t)\mu_5(t), \tag{24}$$

$$\mu_6'(t) - \int_{h_1(t)}^{h_2(t)} x[a(x,t)u_{xx} + b(x,t)u_x + f(x,t)]dx = h_2(t)h_2'(t)u(h_2(t),t) - h_1(t)h_1'(t)u(h_1(t),t) + c(t)\mu_6(t), \tag{25}$$

$$\mu_7'(t) - \int_{h_1(t)}^{h_2(t)} x^2[a(x,t)u_{xx} + b(x,t)u_x + f(x,t)]dx = h_2^2(t)h_2'(t)u(h_2(t),t) - h_1^2(t)h_1'(t)u(h_1(t),t) + c(t)\mu_7(t). \tag{26}$$

Now, evaluating equations (24)–(26) at $t = 0$, we obtain

$$\begin{aligned}
&\mu_2(0)h_2'(0) - \mu_1(0)h_1'(0) + c(0)\mu_5(0) \\
&= \mu_5'(0) - \int_{h_{01}}^{h_{02}} [a(x,0)\phi''(x) + b(x,0)\phi'(x) + f(x,0)]dx =: d_1, \\
&\mu_2(0)h_{02}h_2'(0) - \mu_1(0)h_{01}h_1'(0) + c(0)\mu_6(0) \\
&= \mu_6'(0) - \int_{h_{01}}^{h_{20}} x[a(x,0)\phi''(x) + b(x,0)\phi'(x) + f(x,0)]dx =: d_2, \\
&\mu_2(0)h_{02}^2h_2'(0) - \mu_1(0)h_{01}^2h_1'(0) + c(0)\mu_7(0) \\
&= \mu_7'(0) - \int_{h_{01}}^{h_{02}} x^2[a(x,0)\phi''(x) + b(x,0)\phi'(x) + f(x,0)]dx =: d_3.
\end{aligned}$$

We can summarise these equations as follows:

$$\begin{bmatrix} -\mu_1(0) & \mu_2(0) & \mu_5(0) \\ -\mu_1(0)h_{01} & \mu_2(0)h_{02} & \mu_6(0) \\ -\mu_1(0)h_{01}^2 & \mu_2(0)h_{02}^2 & \mu_7(0) \end{bmatrix} \begin{bmatrix} h_1'(0) \\ h_2'(0) \\ c(0) \end{bmatrix} = \begin{bmatrix} d_1 \\ d_2 \\ d_3 \end{bmatrix}. \tag{27}$$

Solving this system of equations for $h_1'(0)$, $h_2'(0)$ and $c(0)$ we obtain the solution

$$h_1'(0) = \frac{d_3(-h_{02}\mu_5(0) + \mu_6(0)) + d_2\left(h_{02}^2\mu_5(0) - \mu_7(0)\right) + d_1h_{02}(-h_{02}\mu_6(0) + \mu_7(0))}{(h_{01} - h_{02})\mu_1(0)(h_{01}h_{02}\mu_5(0) - h_{01}\mu_6(0) - h_{02}\mu_6(0) + \mu_7(0))}, \tag{28}$$

$$h_2'(0) = \frac{d_3(-h_{01}\mu_5(0) + \mu_6(0)) + d_2\left(h_{01}^2\mu_5(0) - \mu_7(0)\right) + d_1h_{01}(-h_{01}\mu_6(0) + \mu_7(0))}{(h_{01} - h_{02})\mu_2(0)(h_{01}h_{02}\mu_5(0) - h_{01}\mu_6(0) - h_{02}\mu_6(0) + \mu_7(0))}, \tag{29}$$

$$c(0) = \frac{d_3 + d_1h_{01}h_{02} - d_2(h_{01} + h_{02})}{h_{01}h_{02}\mu_5(0) - h_{01}\mu_6(0) - h_{02}\mu_6(0) + \mu_7(0)}. \tag{30}$$

4 Numerical solution of inverse problems

For the inverse problems described in Sections 2 and 3, our aim is the simultaneous stable reconstructions of the time-dependent unknown coefficient $c(t)$, together with the unknown moving boundaries $h_1(t)$ and $h_3(t)$, and the transformed temperature $v(y,t)$, satisfying the equations (8)-(13) or, (8)-(10), (13), (19) and (20). This is accomplished by minimizing the following nonlinear least-squares Tikhonov regularization functionals:

$$\begin{aligned}
F_1(h_1, h_3, c) = &\left\| h_1'(t) - \frac{v_y(0,t)}{h_3(t)} - \mu_3(t) \right\|^2 + \left\| h_3'(t) - \frac{v_y(0,t) + v_y(1,t)}{h_3(t)} + \mu_3(t) - \mu_4(t) \right\|^2 \\
&+ \left\| h_3(t)\int_0^1 v(y,t)dy - \mu_5(t) \right\|^2 + \beta\|c(t)\|^2,
\end{aligned} \tag{31}$$

$$\begin{aligned}
F_2(h_1, h_3, c) = &\left\| h_3(t)\int_0^1 v(y,t)dy - \mu_5(t) \right\|^2 + \left\| h_3^2(t)\int_0^1 yv(y,t)dy + h_1(t)\mu_5(t) - \mu_6(t) \right\|^2 \\
&+ \left\| h_3^3(t)\int_0^1 y^2v(y,t)dy - h_1^2(t)\mu_5(t) + 2h_1(t)\mu_6(t) - \mu_7(t) \right\|^2 + \beta\|c(t)\|^2,
\end{aligned} \tag{32}$$

where $\beta \geq 0$ is a regularization parameter penalising the coefficient $c(t)$, the norm is in the space $L^2[0,T]$, and v solves the direct problem (8)–(10) for given (h_1, h_3, c). We have also investigated penalising the free boundaries $h_1(t)$ and $h_3(t)$ with positive regularization parameters, but the results obtained with no regularization were obtained already stable, indicating that the inverse problem is ill-posed (unstable) in the components $c(t)$, but not in the other component $h_1(t)$, $h_3(t)$ and $v(y,t)$.

The discretised form of equations (31) and (32) are

$$
\begin{aligned}
F_1(\underline{h}_1, \underline{h}_3, \underline{c}) = & \sum_{j=1}^{N} \left[h_1'(t_j) - \frac{v_y(0,t_j)}{h_3(t_j)} - \mu_3(t_j) \right]^2 \\
& + \sum_{j=1}^{N} \left[h_3'(t_j) - \frac{v_y(0,t_j) + v_y(1,t_j)}{h_3(t_j)} + \mu_3(t_j) - \mu_4(t_j) \right]^2 \\
& + \sum_{j=1}^{N} \left[h_3(t_j) \int_0^1 v(y,t_j)dy - \mu_5(t_j) \right]^2 + \beta \sum_{j=1}^{N} c^2(t_j),
\end{aligned} \tag{33}
$$

$$
\begin{aligned}
F_2(\underline{h}_1, \underline{h}_3, \underline{c}) = & \sum_{j=1}^{N} \left[h_3(t_j) \int_0^1 v(y,t_j)dy - \mu_5(t_j) \right]^2 \\
& + \sum_{j=1}^{N} \left[h_3^2(t_j) \int_0^1 yv(y,t_j)dy + h_1(t_j)\mu_5(t_j) - \mu_6(t_j) \right]^2 \\
& + \sum_{j=1}^{N} \left[h_3^3(t_j) \int_0^1 y^2 v(y,t_j)dy - h_1^2(t_j)\mu_5(t_j) + 2h_1(t_j)\mu_6(t_j) - \mu_7(t_j) \right]^2 \\
& + \beta \sum_{j=1}^{N} c^2(t_j),
\end{aligned} \tag{34}
$$

respectively, where $t_j = jT/N$ for $j = \overline{1,N}$. The minimization of F_1, or F_2 is performed using the MATLAB optimization toolbox routine *lsqnonlin*, which does not require the user to supply the gradient of the objective function, [10]. This routine attempts to find the minimum of a sum of squares by starting from an arbitrary initial guesses, subject to the physical constraint $h_3(t) > 0$. Thus, we take the lower and upper simple bounds for $h_3(t)$ to be 10^{-8} and 10^3 and the lower and upper bounds for $h_1(t)$ and $c(t)$ to be -10^3 and 10^3, respectively. Furthermore, within *lsqnonlin*, we use the Trust Region Reflective (TRR) algorithm [11], which is based on the interior-reflective Newton method. We also take the parameters of the routine as follows:

- Maximum number of iterations, (MaxIter) $= 10\times$ (number of variables).
- Maximum number of objective function evaluations, (MaxFunEvals) $= 10^5\times$ (number of variables).
- Termination tolerance on the function value, (TolFun) $= 10^{-15}$.
- Solution tolerance, (XTol) $= 10^{-15}$.

The expressions (21) and (22) can be approximated using the following finite difference approximation formulas and trapezoidal rule for integrals:

$$\mu_3(t_j) = \frac{h_{1j} - h_{1j-1}}{\Delta t} - \frac{4v_{1,j} - v_{2,j} - 3v_{0,j}}{2(\Delta y)h_{3j}}, \quad j = \overline{1, N}, \tag{35}$$

$$\mu_4(t_j) = \frac{h_{3j} - h_{3j-1}}{\Delta t} - \left(\frac{4v_{1,j} - v_{2,j} - 3v_{0,j}}{2(\Delta y)h_{3j}} - \frac{4v_{M-1,j} - v_{M-2,j} - 3v_{M,j}}{2(\Delta y)h_{3j}} \right) + \mu_3(t_j), \quad j = \overline{1, N}, \tag{36}$$

$$\mu_{\ell+4}(t_j) = \frac{h^{\ell}_{3j}}{2N} \left(y_0^{\ell-1} v_{0,j} + y_M^{\ell-1} v_{M,j} + 2 \sum_{i=1}^{M-1} y_i^{\ell-1} v_{i,j} \right), \quad j = \overline{1, N}, \ \ell = 1, 2, 3, \tag{37}$$

where $\Delta t = T/N$ and $\Delta y = 1/M$.

Remark. The direct problem (8)-(13) was solved in detail in [1]. The numerical solution for the transformed temperature $v(y, t)$ was obtained in excellent agreement with the exact solution (45) and hence it is not presented here.

In order to model the errors in the measured data, we replace $\mu_{\ell+2}(t_j)$ for $\ell = \overline{1, 5}$, in equations (11)-(13) or, (21)-(22) by $\mu^{\epsilon\ell}_{\ell+2}(t_j)$, by

$$\mu^{\epsilon\ell}_{\ell+2}(t_j) = \mu_{\ell+2}(t_j) + \epsilon\ell_j, \quad \ell = \overline{1, 5}, \ j = \overline{1, N}, \tag{38}$$

where $\epsilon\ell_j$ are random variables generated from a Gaussian normal distribution using the MATLAB function *normrnd* as:

$$\epsilon\ell = normrnd(0, \sigma_\ell, N), \quad \ell = \overline{1, 5}, \tag{39}$$

with mean zero and standard deviation $\sigma_\ell = p \times \max_{t \in [0,T]} \left| \mu_{\ell+2}(t) \right|$ for $\ell = \overline{1, 5}$, where p represents the percentage of noise.

5 Numerical results and discussion

In this section, we present a couple of benchmark numerical test examples to illustrate the accuracy and stability of the numerical methods based on the finite-difference method (FDM) based on the Crank-Nicolson scheme (mesh size $\Delta y = 1/M$, $\Delta t = T/N$ with $M = N = 40$ and taking $T = 2$) combined with the minimization of the objective function F_1 or F_2, as described in Section 4. Furthermore, we add noise to the input measurement data (11)-(13) and (21)-(22) to simulate the real situation of errors in measurements, by using equations (38) and (39). To examine the accuracy of the numerical solution, we use the root mean squares error (*rmse*) defined by

$$rmse(\underline{h}_1) = \left[\frac{T}{N} \sum_{j=1}^{N} (h_1^{Numerical}(t_j) - h_1^{Exact}(t_j))^2 \right]^{1/2}, \tag{40}$$

and similar expessions exist for $\underline{h}_3$ and $\underline{c}$. All numerical computations have been carried out on a Laptop with CPU 2.70 Hertz and RAM 16GB on MATLAB @2017a.

5.1 Example 1 (for inverse problem (8)–(13))

Consider the inverse problem (8)–(13) with unknown coefficients $h_1(t)$, $h_2(t)$ and $c(t)$, and the following input data:

$$
\begin{aligned}
&a(x,t) = 1, \quad b(x,t) = t(1+x), \quad \phi(x) = \pi + \tan^{-1}(x),\\
&\mu_1(t) = (1+t)\left(\pi + \tan^{-1}\left(\frac{5+t}{10}\right)\right), \quad \mu_2(t) = (1+t)\left(\pi + \tan^{-1}\left(\frac{15+2t}{10}\right)\right),\\
&f(x,t) = \pi + \frac{2(1+t)}{(1+x^2)^2} - \frac{t(1+t)(1+x)}{1+x^2} + \tan^{-1}(x) + (1+t)^2(\pi + \tan^{-1}(x)),\\
&\mu_3(t) = \frac{1}{10} - \frac{100(1+t)}{125+10t+t^2}, \quad \mu_4(t) = \frac{825+560t+4t^2}{1625+300t+20t^2} \qquad (41)\\
&\mu_5(t) = \frac{1+t}{10}\left(10\pi + \pi t + (15+2t)\tan^{-1}\left(\frac{15+2t}{10}\right) - (5+t)\tan^{-1}\left(\frac{5+t}{10}\right)\right.\\
&\quad \left. + 5\ln\left(\frac{125+10t+t^2}{325+60t+4t^2}\right)\right), \qquad (42)\\
&\mu_6(t) = \frac{1+t}{200}\left((10+t)(-10+20\pi+3\pi t) + (325+60t+4t^2)\tan^{-1}\left(\frac{15+2t}{10}\right)\right.\\
&\quad \left. - (125+10t+t^2)\tan^{-1}\left(\frac{5+t}{10}\right)\right), \qquad (43)\\
&\mu_7(t) = \frac{1+t}{3000}\left(-1000 + 3250\pi + 250t + 1275\pi t - 15t^2 + 165\pi t^2 + 7\pi t^3\right.\\
&\quad + (15+2t)^3\tan^{-1}\left(\frac{15+2t}{10}\right) - (5+t)^3\tan^{-1}\left(\frac{5+t}{10}\right)\\
&\quad \left. - 500\ln\left(\frac{125+10t+t^2}{325+60t+4t^2}\right)\right). \qquad (44)
\end{aligned}
$$

One can easily check that the conditions of Theorem 2 hold and hence, the uniqueness of the solution is guaranteed. In fact, one can easily check that the exact solution of the transformed inverse problem (8)-(13) is given by

$$v(y,t) = u(yh_3(t)+h_1(t),t) = (1+t)\left(\pi + \tan^{-1}\left(\frac{5+t+10y+ty}{10}\right)\right), \qquad (45)$$

$$h_1(t) = \frac{5+t}{10}, \quad h_3(t) = \frac{10+t}{10}, \quad c(t) = -1-t. \qquad (46)$$

Also,

$$u(x,t) = (1+t)(\pi + \tan^{-1}(x)). \qquad (47)$$

We take the initial guesses for the vectors $\underline{h}_1$, $\underline{h}_3$ and $\underline{c}$ as follows:

$$h^0_{1j} = h_{01} = 0.5, \quad h^0_{3j} = h_{02} - h_{01} = 1, \quad c^0_j = c(0) = -1, \qquad j = \overline{1,N}. \qquad (48)$$

Note that the value of $c(0)$ is known from equation (17).

Let us start our investigation for the recovery of the unknowns $\underline{h}_1$, $\underline{h}_3$ and $\underline{c}$, when there is no noise in the measured data (11)-(13), i.e., $p = 0$, and no regularization applied, i.e, $\beta = 0$. The unregularised objective function F_1, as a function of the number of iterations, is plotted in Figure 1. From this figure, one can notice that a rapid monotonically decreasing convergence to a very low value of order $O(10^{-9})$ is achieved in 9 iterations (in less than 20 minutes of computational time). In fact, the minimization routine *lsqnonlin* is stopped because the final change in the sum of squares is less than the selected value of the termination tolerance TolFun $= 10^{-15}$.

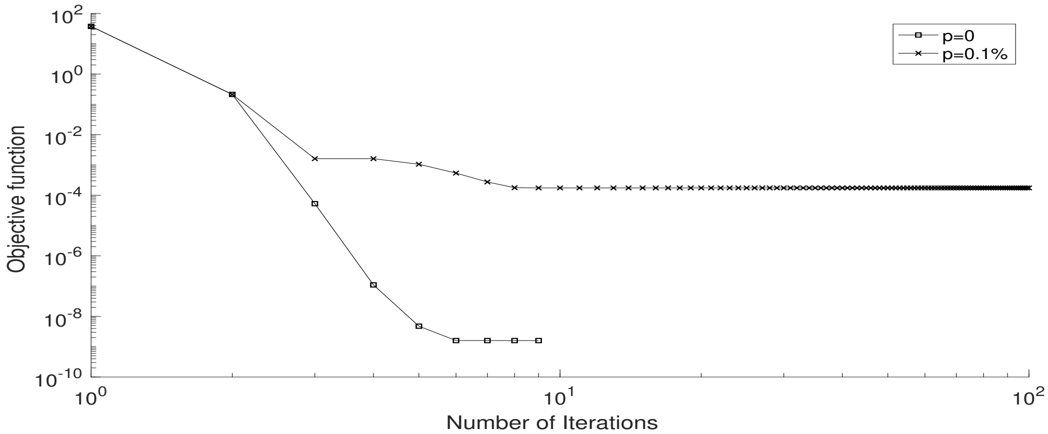


Figure 1: Unregularized objective function (33), for $p \in \{0, 0.1\%\}$ noise and no regularization, for Example 1.

Figure 2 shows the numerical results and the *rmse*, as functions of the number of iterations, for the unknowns $h_1(t)$, $h_3(t)$ and $c(t)$. It can be seen that accurate and stable solutions are obtained. In comparison with the exact solutions we find that at convergence, $rmse(h_1) = 3.6E-4$, $rmse(h_3) = 1.3E-4$ and $rmse(c) = 4.7E-2$, which indicate an excellent agreement. In Figure 2(c) it can be seen that slight instabilities start to appear near the final time $T = 2$. This behaviour is expected since the inverse problem under consideration is ill-posed and less information about $c(t)$ than about $h_1(t)$ and $h_2(t)$ appear in the input data (11)–(13).

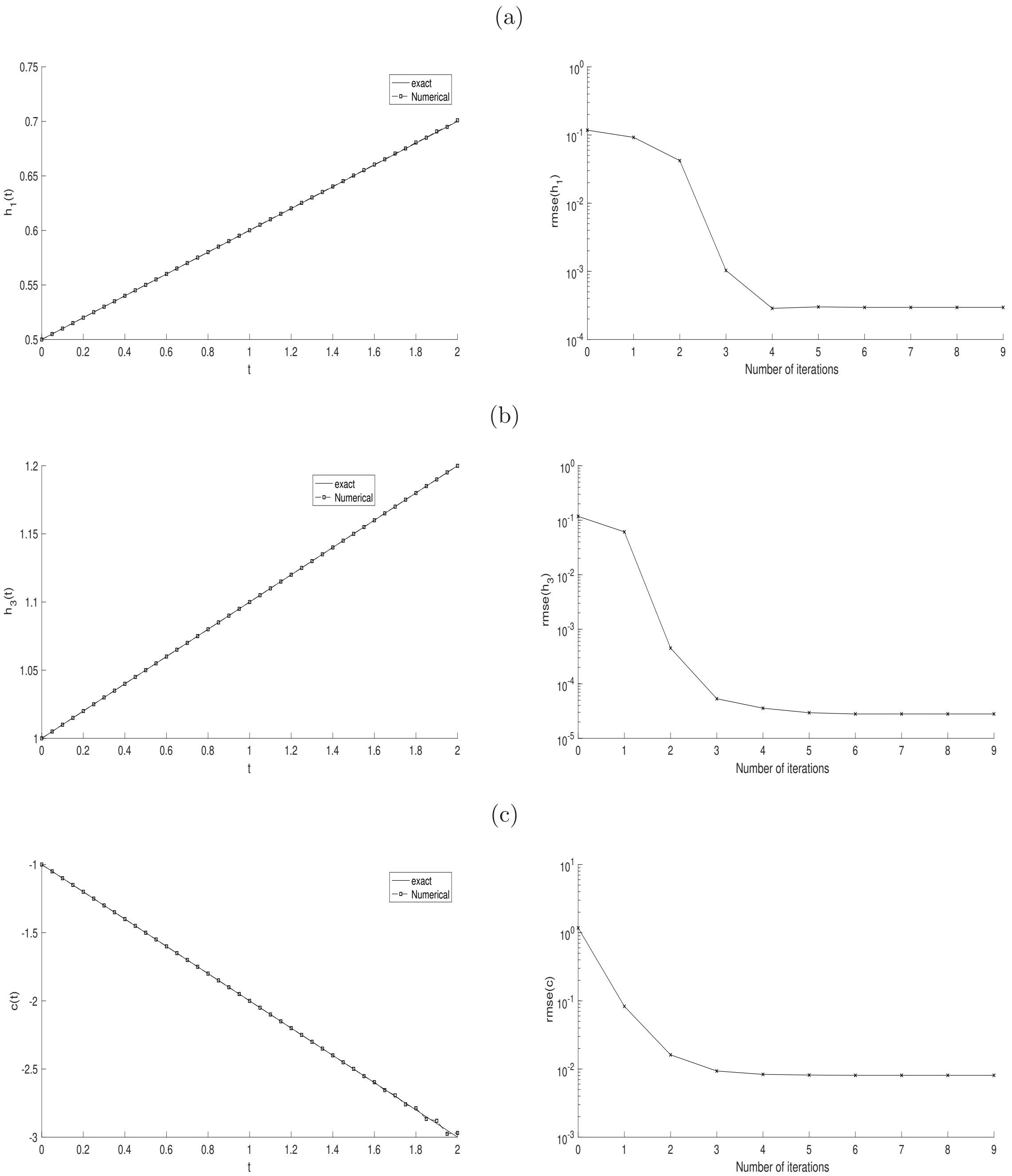


Figure 2: (a) The exact and numerical solutions for: (a) $h_1(t)$, (b) $h_3(t)$ and (c) $c(t)$, for no noise and no regularization, for Example 1, along with the $rmse$ values, as functions of the number of iterations.

The true solution (45) and the numerically obtained solutions for the transformed temperature $v(y, t)$, in the case of no noise and no regularization, are shown in Figure 3.

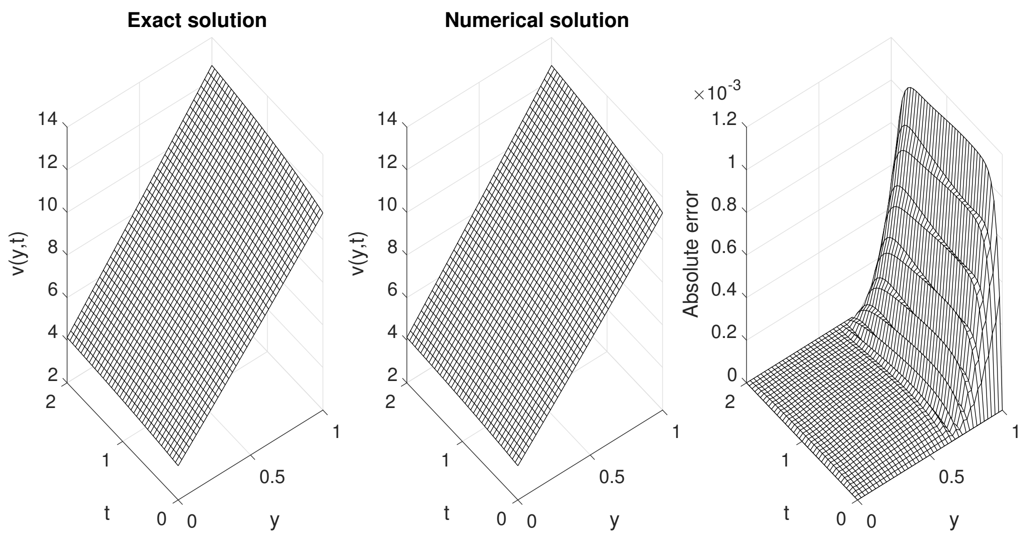


Figure 3: The exact (45) and numerical solutions for the transformed temperature $v(y,t)$, for no noise and no regularization, for Example 1. The absolute error is also included.

Next, we add $p = 0.1\%$ noise in the input data μ_3, μ_4 and μ_5, using (38) and (39). The unregularized objective function F_1 with, $\beta = 0$ is presented in Figure 1. From this figure one can see that a monotonic decreasing achieved in 100 iterations to reach a low value of order $O(10^{-3})$. Also, the associated numerical results presented in Figure 4 are found stable and accurate for h_1 and h_2 (with $rmse(h_1) = 0.0065$, $rmse(h_3) = 2E-3$), but unstable and inaccurate for the coefficient $c(t)$ (with $rmse(c) = 0.4357$). This shows that the inverse problem under investigation is ill-posed problem and small errors (noise) in input data lead to drastic errors in the output coefficient $c(t)$. One can notice that the free boundaries $h_1(t)$ and $h_3(t)$ are not affected by noise inclusion and still have stable features. Therefore, the free boundaries do not need to be regularized. In order to restore the stability of the coefficient $c(t)$, regularization should be applied. We use the Tikhonov regularization method by adding the penalty term in equation (31). We use various regularization parameter values $\beta \in \{10^{-i}$ for $i = \overline{1,8}\}$. For the proper choice of the reqularization parameter we use the L-curve criterion which is a plot (on ordinary or doubly-logarithmic scale) of the norm of the regularized solution versus the residual norm, [3]. This is shown in Figure 5, by plotting the solution norm $\sqrt{\|h_1\|^2 + \|h_3|^2 + \|c\|^2}$ versus the residual norm given by square root of the sum of the first three terms in the right-hand side of equation (31). From this figure, it can be observed that the regularization parameters near the corner of the L-curve are $\beta \in \{10^{-3}, 10^{-2}, 10^{-1}\}$ for $p = 0.1\%$. The optimal choice of regularization parameter based on L-curve criterion is $\beta = 10^{-3}$. This value is also associated with the lowest $rmse$ values for h_1 and h_3 of 5.9E-3 and 1.4E-3, respectively. A low value of $rmse(c) = 0.1976$ is also obtained for $\beta = 10^{-3}$.

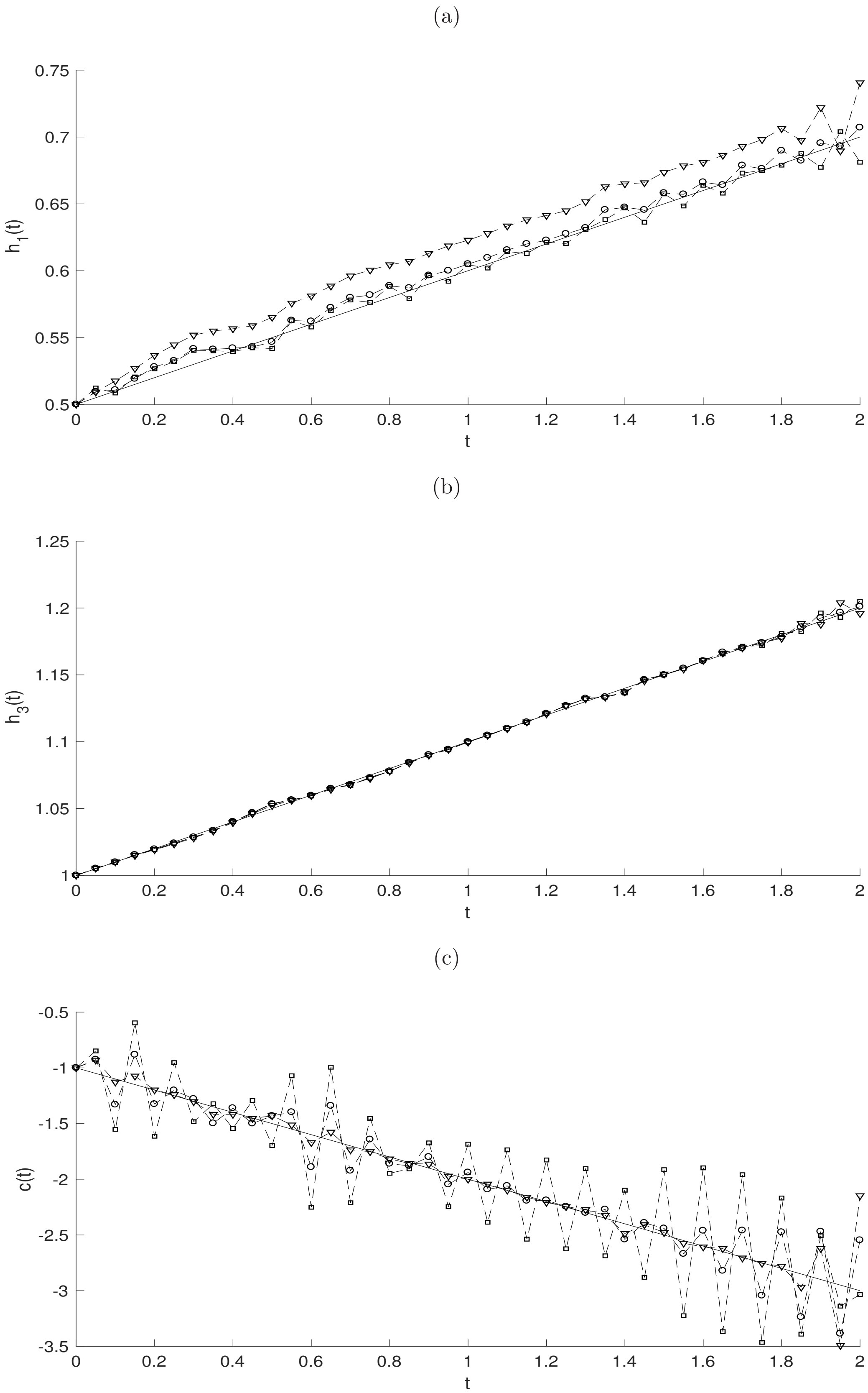
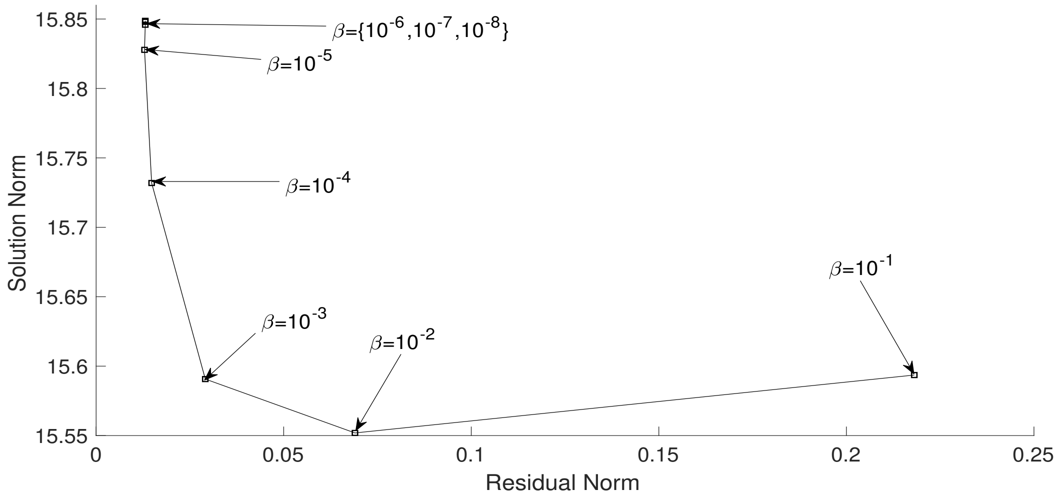


Figure 4: The exact solution (−−−) and numerical solutions without regularization (-□-) and with regularization parameters $\beta = 10^{-3}$ (-○-), $\beta = 10^{-2}$ (-▽-), for $p = 0.1\%$ noise, for: (a) $h_1(t)$, (b) $h_3(t)$ and (c) $c(t)$, for Example 1.

(a)



(b)

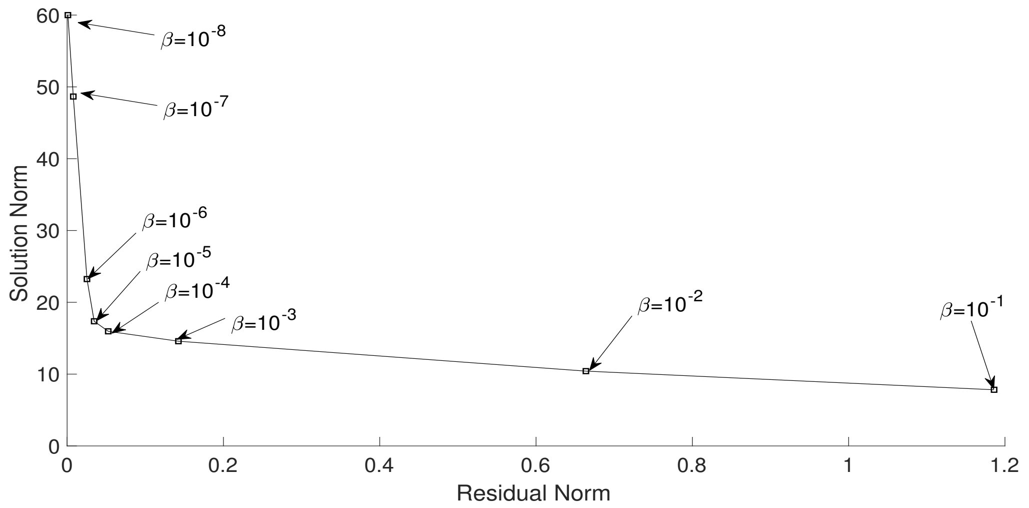


Figure 5: The L-curve method for various regularization parameters, for $p = 0.1\%$ noise, for (a) Example 1 and (b) Example 2.

More numerical details about the objective function values, number of iterations, $rmse$ for unknowns coefficients with various regularization parameters and the computational time are given in Table 1.

Table 1: Numerical results for various regularization parameters $\beta = 0$ and $\beta \in \{10^{-i} | i = 1, ..., 7\}$ for $p = 0.1\%$ noise, for Example 1.

Regularization parameter β								
	0	10^{-7}	10^{-6}	10^{-5}	10^{-4}	10^{-3}	10^{-2}	10^{-1}
No. of iterations	26	72	49	40	43	29	32	35
No. of function evaluations	3348	9052	6200	5084	5456	3720	4092	4464
Objective function (33) value at final iteration	1.7E-4	1.9E-4	3.5E-4	0.0200	0.0184	0.1793	1.7619	17.370
$rmse(h_1)$	8.8E-3	6.3E-3	6.3E-3	6.1E-3	5.3E-3	5.9E-3	0.0219	0.1034
$rmse(h_3)$	2.5E-3	2.0E-3	2.0E-3	1.9E-3	1.7E-3	1.4E-3	2.1E-3	4.9E-3
$rmse(c)$	0.4357	0.4423	0.4411	0.4266	0.3414	0.1976	0.1710	0.1999
Computational time in hours	0.4	5.7	3.9	3.1	3.3	2.3	2.6	1.0

Table 2: Numerical results for various regularization parameters $\beta = 0$ and $\beta \in \{10^{-i} | i = 0, ..., 6\}$ for $p = 1\%$ noise, for Example 1.

Regularization parameter β								
	0	10^{-6}	10^{-5}	10^{-4}	10^{-3}	10^{-2}	10^{-1}	1
No. of iterations	401	401	401	401	401	45	40	46
No. of function evaluations	49848	49848	49848	49848	49848	5704	5084	5828
Objective function (33) value at final iteration	0.0782	0.0790	0.086	0.1451	0.4093	1.9533	15.314	140.202
$rmse(h_1)$	0.4571	0.4580	0.4626	0.2699	0.0773	0.2060	0.3538	0.5354
$rmse(h_3)$	0.0203	0.0203	0.0207	0.0170	0.0155	0.0131	0.0127	0.0166
$rmse(c)$	4.1582	4.1497	4.0283	2.8435	1.3896	0.4308	0.2875	0.3539
Computational time in hours	24.78	24.78	24.78	24.78	24.78	1.03	0.95	0.99

Noisy data μ_3, μ_4 and μ_5 contaminated by a higher amount of noise such as $p = 1\%$ have also been inverted and the numerically obtained results are presented in Figures 6 and 7, and Table 2. From these illustrations it can be observed that stable retrievals of the unknown quantities of interest are obtained for $\beta \in \{10^{-2}, 10^{-1}\}$.

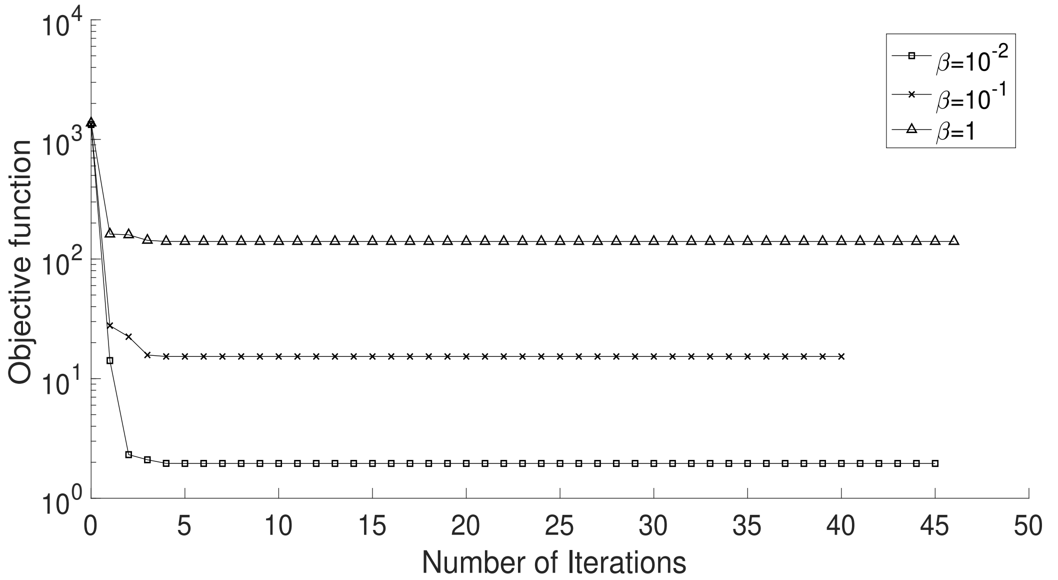
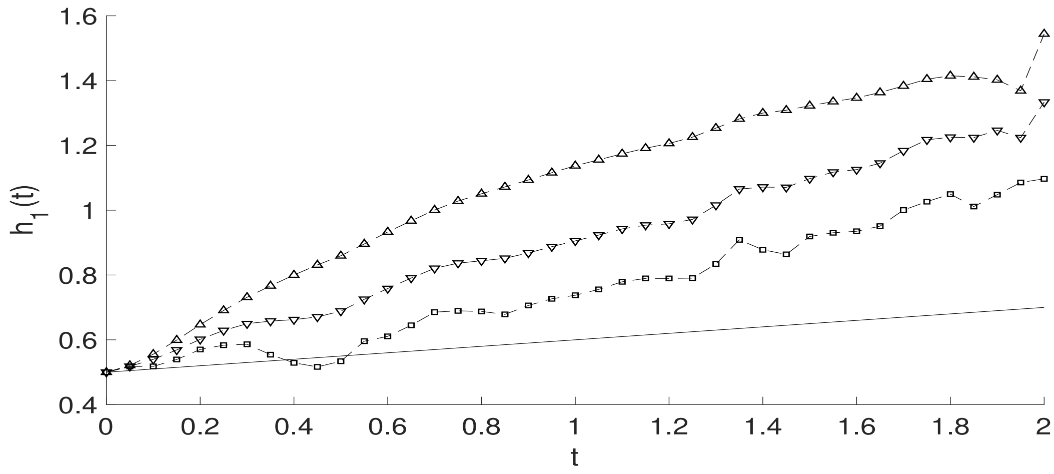
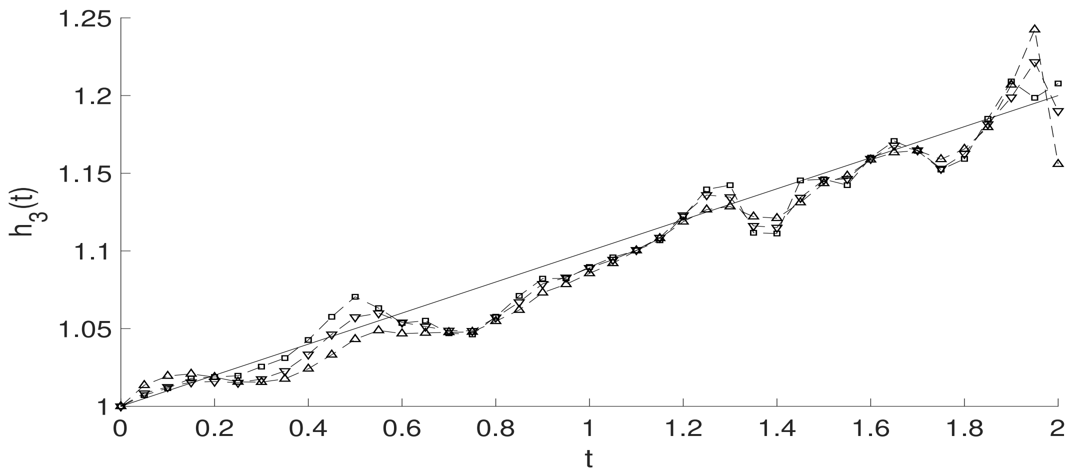


Figure 6: Regularized objective function (33), for $p = 1\%$ noise, for Example 1.

(a)



(b)



(c)

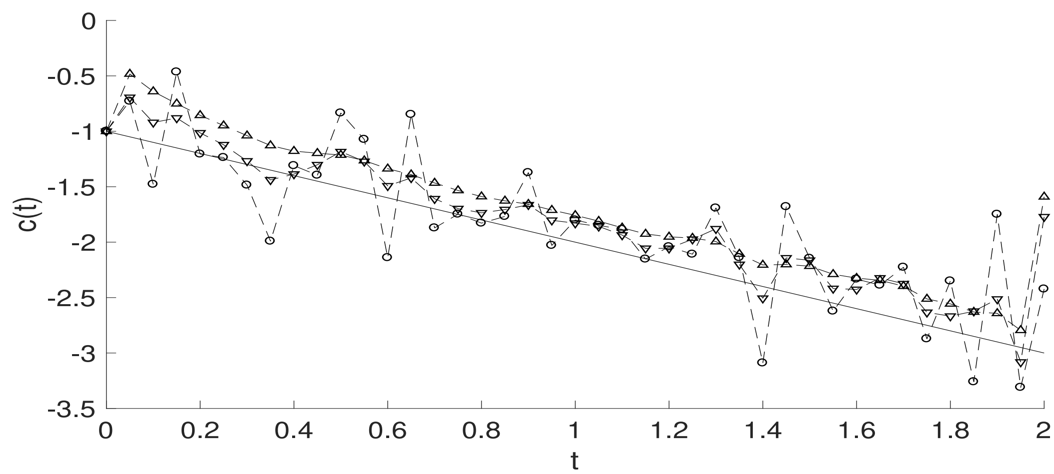


Figure 7: The exact solution $(---)$ and numerical solutions with regularization parameters $\beta = 10^{-2}$ (-□-), $\beta = 10^{-1}$ (-▽-) and $\beta = 1$ (-△-), for $p = 1\%$ noise, for: (a) $h_1(t)$, (b) $h_3(t)$ and (c) $c(t)$, for Example 1.

5.2 Example 2 (for inverse problem II)

We consider the other inverse problem described in Section 3 where we replace the Stefan conditions (4) and (5) by the first- and second-order heat moment measurements (19) and (20), respectively. The input data are the same as in Example 1, but we replace $\mu_3(t)$ and $\mu_4(t)$ by $\mu_6(t)$ and $\mu_7(t)$, computed by equations (43) and (44), respectively. One can easily check that the conditions of Theorem 4 hold and therefore the uniqueness of solution holds. The exact solution is given by equations (45)-(47).

The initial guesses for the values $\underline{h}_1$, $\underline{h}_3$ and $\underline{c}$ are given by (48), with the mention that the value of $c(0)$ is known from equation (30). In order to avoid repetition we only illustrate the results for $p = 0.1\%$ noise in Figure 8 and Table 3. Similar conclusions to those obtained in Figure 4 and Table 1 for Example 1 can be observed.

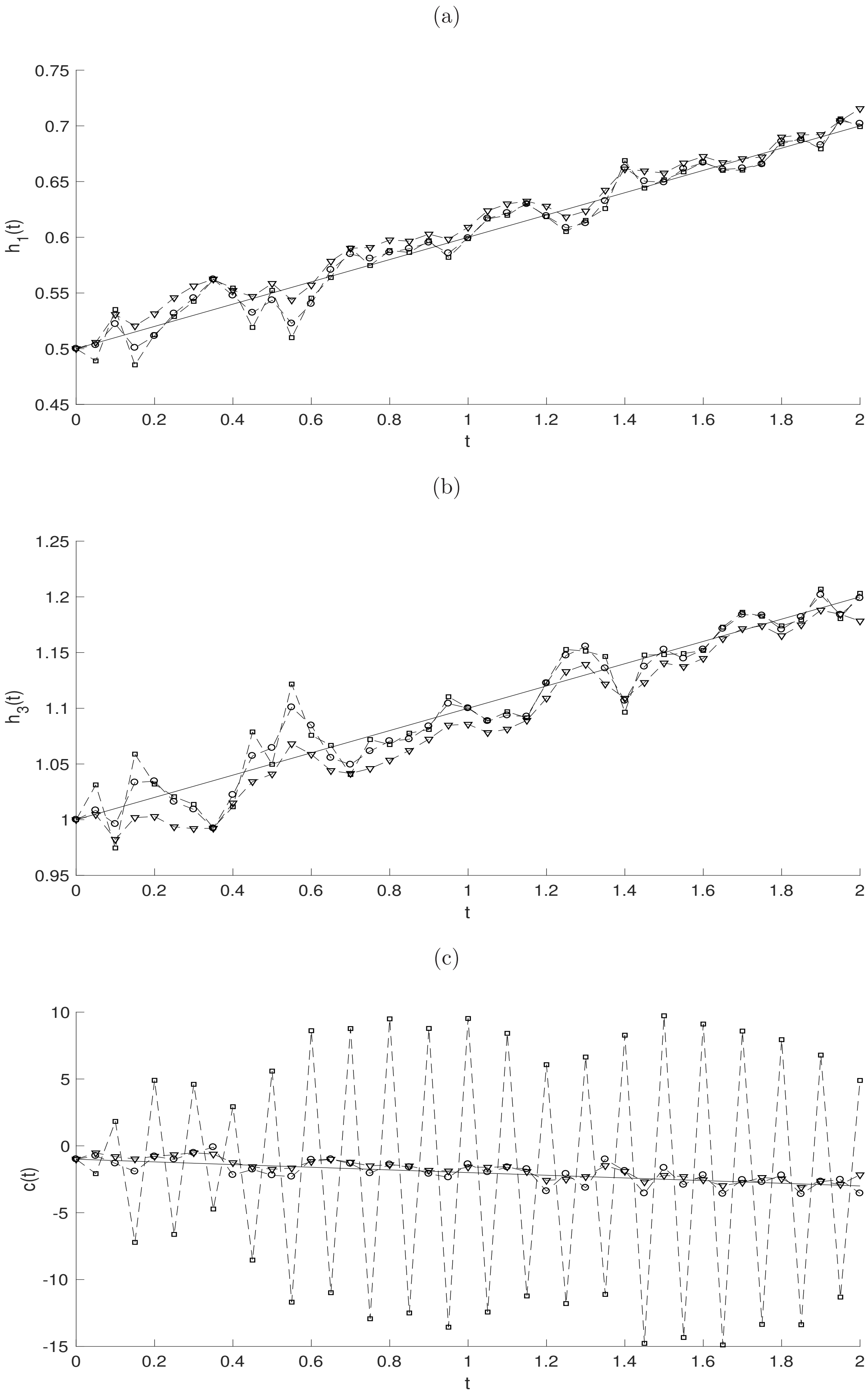


Figure 8: The exact solution (———) and numerical solutions without regularization (-□-) and with regularization parameters $\beta = 10^{-4}$ (-○-), $\beta = 10^{-3}$ (-▽-), for $p = 0.1\%$ noise, for: (a) $h_1(t)$, (b) $h_3(t)$ and (c) $c(t)$, for Example 2.

Table 3: Numerical results for various regularization parameters $\beta = 0$ and $\beta \in \{10^{-i}|i = 1, ..., 7\}$ for $p = 0.1\%$ noise, for Example 2.

Regularization parameter β								
	0	10^{-7}	10^{-6}	10^{-5}	10^{-4}	10^{-3}	10^{-2}	10^{-1}
No. of iterations	29	43	34	20	22	30	32	31
No. of function evaluations	3720	5456	4340	2604	2852	3844	4092	3968
Objective function (34) value at final iteration	4.9E-17	2.9E-4	1.1E-3	3.5E-3	2.1E-2	0.16915	0.916	1.6346
$rmse(h_1)$	0.0151	0.0147	0.0140	0.0133	0.0119	0.0133	0.0479	0.0796
$rmse(h_3)$	0.0220	0.0214	0.0204	0.0194	0.0171	0.0201	0.0730	0.1209
$rmse(c)$	9.4612	7.3162	2.7508	1.2052	0.6305	0.4063	1.1280	1.9422
Computational time in hours	0.5	1.2	0.9	0.5	0.5	0.8	0.9	1.2

6 Conclusions

Inverse problems concerning the simultaneous determination of time-dependent coefficients and free boundaries in the parabolic heat equation have been numerically reconstructed by nonlinear optimization using the MATLAB optimization toolbox routine *lsqnonlin*. From the numerical investigation, the following conclusions can be drawn:

• The process of reconstructing the moving boundaries using the proposed inverse modelling is well-posed. Moreover, the reaction coefficient is (locally) Uniquely solvable, though still ill-posed with respect to small errors in the measured data. To restore stability, regularization has successfully been employed.

• The inverse problem based on measuring the Stefan data (4) and (5) is more stable than that based on measuring the first- and second-order heat moments (19) and (20).

References

[1] Z. Adil and M.S. Hussein (2020) Numerical solution for two-sided Stefan problem, *Iraqi Journal of Science*, **61**, No. 2, 444–452.

[2] J.R. Cannon and J. Van der Hoek (2020) Diffusion subject to the specification of mass, *Journal of Mathematical Analysis and Applications*, **115**, 517–529.

[3] P.C.Hansen, (2001) The L-curve and its use in the numerical treatment of inverse problems. In: *Computational Inverse Problems in Electrocardiology*, (ed. P. Johnston), WIT Press, Southampton, 119-142.

[4] M.J. Huntul and D. Lesnic (2017) Determination of time-dependent coefficients and multiple free boundaries, *Eurasian Journal of Mathematical and Computer Applications*, **5**, 15-43.

[5] M. I. Ivanchov (2012) A problem with free boundary for a two-dimensional parabolic equation, *Journal of Mathematical Sciences*, **183**, No.1, 17–28.

[6] M.I. Ivanchov (2003) Free boundary problem for nonlinear diffusion equation, *Matematychni Studii*, **19**, 156-164.

[7] M.S. Hussein and D. Lesnic (2014) Determination of a time-dependent thermal diffusivity and free boundary in heat conduction, *International Communications in Heat and Mass Transfer*, **53**, 154-163.

[8] M.S. Hussein, D. Lesnic and M.I. Ivanchov (2013) Free boundary determination in nonlinear diffusion. *East Asian Journal on Applied Mathematics*, **3**, No.4, 295-310.

[9] M.S. Hussein, D. Lesnic, M.I. Ivanchov and H.A. Snitko (2016) Multiple time-dependent coefficient identification thermal problems with a free boundary, *Applied Numerical Mathematics*, **99**, 24-50.

[10] Mathwoks. Documentation optimization toolbox, www.mathworks.com, September 2012.

[11] J.J. Moré and D.C. Sorensen (1983) Computing a trust region step, *SIAM Journal on Scientific and Statistical Computing*, **4**, 553-572.

[12] H.A. Snitko (2009) Determination of unknown coefficient in the parabolic equation in the area with free boundary, *Bulletin of Donetsk National University. Series A: Natural Sciences*, **1**, 60-67.