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Multiple time-dependent coefficient identification thermal problems with a free boundary

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Abstract

Multiple time-dependent coefficient identification thermal problems with an unknown free boundary are investigated. The difficulty in solving such inverse and ill-posed free boundary problems is amplified by the fact that several quantities of physical interest (conduction, convection/advection and reaction coefficients) have to be simultaneously identified. The additional measurements which render a unique solution are given by the heat moments of various orders together with a Stefan boundary condition on the unknown moving boundary. Existence and uniqueness theorems are provided. The nonlinear and ill-posed problems are numerically discretised using the finite-difference method and the resulting system of equations is solved numerically using the MATLAB toolbox routine *lsqnonlin* applied to minimizing the nonlinear Tikhonov regularization functional subject to simple physical bounds on the variables. Numerically obtained results from some typical test examples are presented and discussed in order to illustrate the efficiency of the computational methodology adopted.

Keywords: Inverse problem; Tikhonov regularization; Free boundary; Heat equation.

1 Introduction

Inverse coefficient identification problems (ICIP) for partial differential equations are some of the most complicated and practically important problems. Being in addition nonlinear, optimization techniques are mainly used for their numerical solutions, as well as various modifications tailored to the properties of the corresponding direct problems (monotonicity or/and smoothness of their solutions, etc.), [13]. ICIP's with one or several unknown coefficients play a substantial role in the theory and application of inverse problems. A great attention was paid to this kind of inverse problems due to the industrial applications in practice, for instance, the determination of the thermal conductivity, heat capacity, absorption coefficient, etc., in the field of heat conduction or porous media.

Many practical problems involve a free boundary and the Stefan problem is a typical example of a problem of this kind, [22, 23]. Under suitable changes of variables, free boundary problems can be reduced to ICIP's in a fixed domain. This approach opens the new and more complicated area of inverse problems that combine free boundary problems with coefficient identification problems. One of the main feature of these problems is that the unknowns depend solely on the time variable and this enables a neat mathematical treatment based on Green's functions, [11].

Prior to this study, references [4, 6, 10] investigated both theoretically and numerically several such combined formulations for the retrieval of the free boundary together with the thermal diffusivity both which are unknown time-dependent functions. The theoretical investigation has been extended recently to the case of several multiple coefficients in [18, 19] and it the purpose of this study to, apart from some theoretical clarifications which are elaborated in Section 2, perform the numerical realization using the finite-difference method (FDM) combined with a nonlinear least-squares toolbox MATLAB routine, see Sections 3 and 4. In Section 5, we provide numerical results and discussion, whilst Section 6 presents an extension to a triple unknown coefficient identification. Finally, conclusions are highlighted in Section 7.

2 Mathematical formulation

Consider the one-dimensional time-dependent heat equation

$$\frac{\partial u}{\partial t}(x, t) = a(x, t) \frac{\partial^2 u}{\partial x^2}(x, t) + b(t) \frac{\partial u}{\partial x}(x, t) + c(t)u(x, t) + f(x, t), \quad (x, t) \in \Omega \quad (1)$$

for the unknown temperature $u(x, t)$ in the domain $\Omega = \{(x, t) | 0 < x < h(t), 0 < t < T < \infty\}$ with unknown free smooth boundary $x = h(t) > 0$ and time-dependent coefficients $b(t)$ and $c(t)$ representing the convection/advection and reaction coefficients, respectively. Also in (1), $f(x, t)$ represents a given heat source, whilst $a(x, t) > 0$ is the given thermal diffusivity. In many applications, [6, 19, 24], the thermal diffusivity depends on time only, but here we envisage a more general physical situation in which the thermal conductivity depends on time and the heat capacity depends on space such that their ratio defined as the thermal diffusivity depends on both space and time. To give more physical meaning to the inverse problem, we have in mind a process in which a finite slab is undertaking radioactive decay such that its diffusivity, convection and reaction coefficients are unknown but they depend on time [1, Chap.13], [16]. We finally mention that extensions to cases when the time-dependent heat source is also unknown or when some unknown coefficients may depend on space as well have recently been considered elsewhere, [7, 8].

The initial condition is

$$u(x, 0) = \phi(x), \quad 0 \leq x \leq h(0) =: h_0, \quad (2)$$

where $h_0 > 0$ is given, and the Dirichlet boundary conditions are

$$u(0, t) = \mu_1(t), \quad u(h(t), t) = \mu_2(t), \quad t \in [0, T]. \quad (3)$$

As over-determination conditions we consider, [18],

$$h'(t) + u_x(h(t), t) = \mu_3(t), \quad t \in [0, T], \quad (4)$$

$$\int_0^{h(t)} u(x, t) dx = \mu_4(t), \quad t \in [0, T], \quad (5)$$

$$\int_0^{h(t)} xu(x, t) dx = \mu_5(t), \quad t \in [0, T]. \quad (6)$$

Note that $\mu_4(t)$ and $\mu_5(t)$ represent the specification of the energy or, mass of the heat conducting system and heat momentum, respectively, [2, 9, 15]. Also, equation (4) represents a Stefan interface moving boundary condition.

Now we perform the change of variable $y = x/h(t)$ to reduce the problem (1)–(6) to the following inverse problem for the unknowns $h(t)$, $b(t)$, $c(t)$ and $v(y, t) := u(yh(t), t)$:

$$\frac{\partial v}{\partial t}(y, t) = \frac{a(yh(t), t)}{h^2(t)} \frac{\partial^2 v}{\partial y^2}(y, t) + \frac{b(t) + yh'(t)}{h(t)} \frac{\partial v}{\partial y}(y, t) + c(t)v(y, t) + f(yh(t), t),$$

$$(y, t) \in Q_T \quad (7)$$

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

$$v(y, 0) = \phi(h_0 y), \quad y \in [0, 1], \quad (8)$$

$$v(0, t) = \mu_1(t), \quad v(1, t) = \mu_2(t), \quad t \in [0, T], \quad (9)$$

$$h'(t) + \frac{1}{h(t)} v_y(1, t) = \mu_3(t), \quad t \in [0, T], \quad (10)$$

$$h(t) \int_0^1 v(y, t) dy = \mu_4(t), \quad t \in [0, T], \quad (11)$$

$$h^2(t) \int_0^1 yv(y, t) dy = \mu_5(t), \quad t \in [0, T]. \quad (12)$$

A variant of the theorem proved in [18] (under the additional assumption that $h(0) = h_0 > 0$ is known) ensures the unique solvability (locally in time) of the inverse problem (7)–(12), as follows.

Theorem 1. *Suppose that:*

$0 < a \in C^{2,0}([0, \infty) \times [0, T])$, $[0, f_0] \ni f \in C^{1,0}([0, \infty) \times [0, T])$, where $f_0 \geq 0$ is a given constant, $0 < \phi \in C^1[0, h_0]$, $0 < \mu_i \in C^1[0, T]$ for $i = 1, 2, 4, 5$, $\mu_3 \in C[0, T]$,

$$(\mu_2(0) - \mu_1(0))\mu_5(0) - (h_0\mu_2(0) - \mu_4(0))\mu_4(0) \neq 0, \quad (13)$$

$\phi(0) = \mu_1(0)$, $\phi(h_0) = \mu_2(0)$, $\int_0^{h_0} \phi(x) dx = \mu_4(0)$, and $\int_0^{h_0} x\phi(x) dx = \mu_5(0)$. Then, there is $T_0 \in (0, T]$, such that there exists a unique solution $(h(t), b(t), c(t), v(y, t)) \in C^1[0, T_0] \times (C[0, T_0])^2 \times (C^{2,1}(Q_{T_0}) \cap C^{1,0}(\overline{Q_{T_0}}))$, $h(t) > 0$ for $t \in [0, T_0]$, of the inverse problem (7)–(12).

Remarks.

(i) During the computation we need the values of $b(0)$ and $c(0)$. One can derive these values from the governing equation (1) with the help of overdetermination conditions (5) and (6), as follows. Integrating (1) with respect to x over the interval $[0, h(t)]$ we have

$$\int_0^{h(t)} u_t(x, t) dx = a(h(t), t)u_x(h(t), t) - a(0, t)u_x(0, t) - \int_0^{h(t)} a_x(x, t)u_x(x, t) dx$$

$$+ b(t)(\mu_2(t) - \mu_1(t)) + c(t)\mu_4(t) + \int_0^{h(t)} f(x, t) dx. \quad (14)$$

Also, multiplying (1) by x and integrating with respect to x over the interval $[0, h(t)]$, and invoking the integration by parts, we obtain

$$\int_0^{h(t)} xu_t(x, t) dx = h(t)a(h(t), t)u_x(h(t), t) - \int_0^{h(t)} (a(x, t) + xa_x(x, t))u_x(x, t) dx$$

$$+ b(t)(h(t)\mu_2(t) - \mu_4(t)) + c(t)\mu_5(t) + \int_0^{h(t)} xf(x, t) dx. \quad (15)$$

Differentiating equations (5) and (6) with respect to t we obtain

$$\int_0^{h(t)} u_t(x, t) dx = \mu'_4(t) - h'(t)\mu_2(t), \quad \int_0^{h(t)} x u_t(x, t) dx = \mu'_5(t) - h(t)h'(t)\mu_2(t). \quad (16)$$

Substituting (16) into (14) and (15) and using $y = x/h(t)$ we obtain

$$\begin{aligned} b(t)(\mu_2(t) - \mu_1(t)) + c(t)\mu_4(t) &= \mu'_4(t) - \mu_2(t)h'(t) + \frac{a(0, t)w(0, t) - a(h(t), t)w(1, t)}{h(t)} \\ &+ \int_0^1 a_x(yh(t), t)w(y, t)dy - h(t) \int_0^1 f(yh(t), t)dy, \end{aligned} \quad (17)$$

$$\begin{aligned} b(t)(h(t)\mu_2(t) - \mu_4(t)) + c(t)\mu_5(t) &= \mu'_5(t) - \mu_2(t)h(t)h'(t) - a(h(t), t)w(1, t) \\ &+ \int_0^1 (a(yh(t), t) + yh(t)a_x(yh(t), t))w(y, t)dy - h^2(t) \int_0^1 yf(yh(t), t)dy, \end{aligned} \quad (18)$$

where we have denoted $w(y, t) := v_y(y, t)$. Equation (10) also gives

$$h'(t) = -\frac{w(1, t)}{h(t)} + \mu_3(t), \quad t \in [0, T]. \quad (19)$$

Substituting this expression into (17) and (18) and solving the resulting system of equations for $b(t)$ and $c(t)$, result in equations (18) and (19) (corrected) of [18], namely,

$$\begin{aligned} b(t) &= \frac{1}{D_1(t)} \left\{ \int_0^1 [(\mu_5(t) - yh(t)\mu_4(t))a_x(yh(t), t) - a(yh(t), t)\mu_4(t)]w(y, t)dy \right. \\ &+ \frac{a(0, t)\mu_5(t)}{h(t)}w(0, t) + \frac{(\mu_2(t) - a(h(t), t))(\mu_5(t) - h(t)\mu_4(t))}{h(t)}w(1, t) \\ &- h(t) \int_0^1 (\mu_5(t) - yh(t)\mu_4(t))f(yh(t), t)dy + \mu'_4(t)\mu_5(t) - \mu_4(t)\mu'_5(t) \\ &\left. - \mu_2(t)\mu_3(t)(\mu_5(t) - h(t)\mu_4(t)) \right\}, \quad t \in [0, T], \end{aligned} \quad (20)$$

$$\begin{aligned} c(t) &= \frac{1}{D_1(t)} \left\{ \int_0^1 [(\mu_2(t) - \mu_1(t))a(yh(t), t) + (h(t)(\mu_2(t)(y - 1) - y\mu_1(t)) \right. \\ &+ \mu_4(t))a_x(yh(t), t)]w(y, t)dy + \frac{(\mu_4(t) - h(t)\mu_2(t))a(0, t)}{h(t)}w(0, t) \\ &+ \frac{(\mu_2(t) - a(h(t), t))(\mu_4(t) - h(t)\mu_1(t))}{h(t)}w(1, t) - h(t)\mu_2(t)(\mu'_4(t) - \mu_1(t)\mu_3(t)) \\ &- h(t) \int_0^1 \left(\mu_4(t) + h(t)(\mu_2(t)(y - 1) - y\mu_1(t)) \right) f(yh(t), t)dy \\ &\left. + \mu_4(t)\mu'_4(t) + \mu'_5(t)(\mu_2(t) - \mu_1(t)) - \mu_2(t)\mu_3(t)\mu_4(t) \right\}, \quad t \in [0, T], \end{aligned} \quad (21)$$

where

$$D_1(t) := (\mu_2(t) - \mu_1(t))\mu_5(t) - (h(t)\mu_2(t) - \mu_4(t))\mu_4(t), \quad t \in [0, T]. \quad (22)$$

One can observe that condition (13) of Theorem 1 is equivalent to $D_1(0) \neq 0$, and since the functions in (22) are continuous in $[0, T]$ we obtain that $D_1(t) \neq 0$ in an upper neighbourhood

$[0, T_1]$ of $t = 0$, where $T_1 \in (0, T]$. So, at least in this neighbourhood the denominator in (20) and (21) does not vanish hence, these expressions are well-defined.

Letting $t = 0$ in the analogue of expressions (20) and (21) in the variable x , we obtain the values of $b(0)$ and $c(0)$ explicitly, as follows:

$$\begin{aligned}
b(0) = & \frac{1}{D_1(0)} \left[\int_0^{h_0} [(\mu_5(0) - x\mu_4(0))a_x(x, 0) - a(x, 0)\mu_4(0)]\phi'(x)dx \right. \\
& + a(0, 0)\mu_5(0)\phi'(0) + (\mu_2(0) - a(h_0, 0))(\mu_5(0) - h_0\mu_4(0))\phi'(h_0) \\
& - \int_0^{h_0} (\mu_5(0) - x\mu_4(0))f(x, 0)dx + \mu_4'(0)\mu_5(0) - \mu_4(0)\mu_5'(0) \\
& \left. - \mu_2(0)\mu_3(0)(\mu_5(0) - h_0\mu_4(0)) \right], \tag{23}
\end{aligned}$$

$$\begin{aligned}
c(0) = & \frac{1}{D_1(0)} \left[\int_0^{h_0} \left((\mu_2(0) - \mu_1(0))a(x, 0) + (\mu_2(0)(x - h_0) - x\mu_1(0) \right. \right. \\
& \left. \left. + \mu_4(0))a_x(x, 0) \right) \phi'(x)dx + a(0, 0)\phi'(0)(\mu_4(0) - h_0\mu_2(0)) \right. \\
& + (\mu_2(0) - a(h_0, 0))(\mu_4(0) - h_0\mu_1(0))\phi'(h_0) - h(0)\mu_2(0)(\mu_4'(0) - \mu_1(0)\mu_3(0)) \\
& - \int_0^{h_0} (\mu_4(0) + \mu_2(0)(x - h_0) - x\mu_1(0))f(x, 0)dx \\
& \left. + \mu_4(0)\mu_4'(0) + \mu_5'(0)(\mu_2(0) - \mu_1(0)) - \mu_2(0)\mu_3(0)\mu_4(0) \right]. \tag{24}
\end{aligned}$$

One can further elaborate on the determinant (22) of the system of equations (14) and (15), by rewriting it as follows:

$$\begin{aligned}
D_1(t) = & \int_0^{h(t)} u_x(x, t)dx \int_0^{h(t)} xu(x, t)dx - \int_0^{h(t)} u(x, t)dx \int_0^{h(t)} xu_x(x, t)dx \\
= & \int_0^{h(t)} \int_0^{h(t)} (\xi - x)u(\xi, t)u_x(x, t)dxd\xi. \tag{25}
\end{aligned}$$

Let us divide the square $(0, h(t)) \times (0, h(t))$ by its main diagonal and separate the integration in (25) into two parts. Then we obtain

$$D_1(t) = - \int_0^{h(t)} dx \int_0^x (x - \xi)u(\xi, t)u_x(x, t)d\xi + \int_0^{h(t)} d\xi \int_0^\xi (\xi - x)u(\xi, t)u_x(x, t)d\xi.$$

In the first integral change x by ξ and ξ by x to obtain

$$\begin{aligned}
D_1(t) = & - \int_0^{h(t)} u_\xi(\xi, t)d\xi \int_0^\xi (\xi - x)u(x, t)dx + \int_0^{h(t)} u(\xi, t)d\xi \int_0^\xi (\xi - x)u_x(x, t)dx \\
= & \int_0^{h(t)} d\xi \int_0^\xi (\xi - x)[u(\xi, t)u_x(x, t) - u(x, t)u_\xi(\xi, t)]dx \\
= & \int_0^{h(t)} u(\xi, t)d\xi \int_0^\xi (\xi - x)u(x, t) \left(\frac{u_x(x, t)}{u(x, t)} - \frac{u_\xi(\xi, t)}{u(\xi, t)} \right) dx \\
= & - \int_0^{h(t)} u(\xi, t)d\xi \int_0^\xi (\xi - x)u(x, t)dx \int_x^\xi \frac{\partial}{\partial \zeta} \left(\frac{u_\zeta(\zeta, t)}{u(\zeta, t)} \right) d\zeta. \tag{26}
\end{aligned}$$

From conditions $\phi > 0$, $\mu_1 > 0$, $\mu_2 > 0$, $f \geq 0$, $a > 0$, it follows from the minimum principle that

$$u(x, t) > 0, \quad (x, t) \in \bar{\Omega}. \quad (27)$$

The last derivative in (26) is given by

$$\frac{\partial^2}{\partial \zeta^2} \left(\ln u(\zeta, t) \right) = \frac{\partial}{\partial \zeta} \left(\frac{u_\zeta(\zeta, t)}{u(\zeta, t)} \right) = \frac{u_{\zeta\zeta}(\zeta, t)}{u(\zeta, t)} - \frac{u_\zeta^2(\zeta, t)}{u^2(\zeta, t)}. \quad (28)$$

One can therefore make $D_1(t) \neq 0$ in (26) if, via (28), we have $(\ln u(\zeta, t))_{\zeta\zeta} \neq 0$. This last inequality may be satisfied locally in time (in a neighborhood of $t = 0$) if $\phi \in C^2[0, h_0]$ and $(\ln \phi)'' \neq 0$.

(ii) If we make the stronger assumption that $\phi \in C^2[0, h_0]$ then, there is a simpler way to obtain $b(0)$ and $c(0)$ in terms of expressions that do not involve the heat moments μ_4 and μ_5 by using the direct problem data (2) and (3) only. Indeed, if we put $(x, t) = (0, 0)$ and $(x, t) = (h_0, 0)$ into equation (1) we obtain

$$\left. \begin{aligned} \mu'_1(0) &= a(0, 0)\phi''(0) + b(0)\phi'(0) + c(0)\phi(0) + f(0, 0), \\ \mu'_2(0) &= a(h_0, 0)\phi''(h_0) + b(0)\phi'(h_0) + c(0)\phi(h_0) + f(h_0, 0). \end{aligned} \right\} \quad (29)$$

Then, provided that $\phi'(0)\phi(h_0) - \phi(0)\phi'(h_0) \neq 0$, the solution of this system is given by

$$b(0) = \frac{\phi(h_0)(\mu'_1(0) - a(0, 0)\phi''(0) - f(0, 0)) - \phi(0)(\mu'_2(0) - a(h_0, 0)\phi''(h_0) - f(h_0, 0))}{\phi'(0)\phi(h_0) - \phi(0)\phi'(h_0)}, \quad (30)$$

$$c(0) = \frac{\phi'(0)(\mu'_2(0) - a(h_0, 0)\phi''(h_0) - f(h_0, 0)) - \phi'(h_0)(\mu'_1(0) - a(0, 0)\phi''(0) - f(0, 0))}{\phi'(0)\phi(h_0) - \phi(0)\phi'(h_0)} \quad (31)$$

(iii) In [18], a stronger assumption than (13) was used. Namely, that

$$(\mu_2(t) - \mu_1(t))\mu_5(t) - (H_1\mu_2(t) - \mu_4(t))\mu_4(t) > 0, \quad t \in [0, T], \quad (32)$$

where

$$H_1 = \frac{2 \max_{t \in [0, T]} \mu_4(t)}{\min \left\{ \min_{x \in [0, h_0]} \phi(x), \min_{t \in [0, T]} \mu_1(t), \min_{t \in [0, T]} \mu_2(t) \right\}}. \quad (33)$$

However, assumption (32) seems too restrictive and it is difficult to ensure in numerical experiments (with an analytical solution available). Whilst the less restrictive condition (13) still ensures the local unique solvability of the inverse problem. Furthermore, expressions (20) and (21) for $b(t)$ and $c(t)$, respectively, are well-defined if the function D_1 defined in (22), does not vanish on the interval $[0, T]$.

Once the unique local solvability to the inverse problem (7)–(12) has been provided by Theorem 1, the next three Sections 3-5 explain, discuss and illustrate the procedures for obtaining an accurate and stable numerical solution. But before we do that, in the next subsection we introduce another related problem in which the Stefan condition (10) is replaced by the second-order heat moment condition (34).

2.1 Another related inverse problem formulation

It was pointed out in [18] that the Stefan condition (4), or (10), may be replaced by the second-order heat moment measurement

$$\int_0^{h(t)} x^2 u(x, t) dx = \mu_6(t), \quad t \in [0, T], \quad (34)$$

or, in terms of the variable $y = x/h(t)$,

$$h^3(t) \int_0^1 y^2 v(y, t) dy = \mu_6(t), \quad t \in [0, T], \quad (35)$$

respectively. Then, we can formulate the following theorem on the local unique solvability of the inverse problem (7)–(9), (11), (12) and (35), which is a variant of Theorem 2 of [18] when $h(0) = h_0 > 0$ is assumed to be known.

Theorem 2. *Suppose that:*

$0 < a \in C^{2,0}([0, \infty) \times [0, T])$, $[0, f_0] \ni f \in C^{1,0}([0, \infty) \times [0, T])$, where $f_0 \geq 0$ is a given constant, $0 < \phi \in C^1[0, h_0]$, $0 < \mu_i \in C^1[0, T]$ for $i = 1, 2, 4, 5, 6$,

$$\mu_4(0)\mu_6(0) - 2\mu_5^2(0) - h_0(\mu_6(0)\mu_1(0) - 2\mu_4(0)\mu_5(0)) - h_0^2(\mu_4^2(0) - \mu_1(0)\mu_5(0)) \neq 0, \quad (36)$$

$\phi(0) = \mu_1(0)$, $\phi(h_0) = \mu_2(0)$, $\int_0^{h_0} \phi(x) dx = \mu_4(0)$, $\int_0^{h_0} x\phi(x) dx = \mu_5(0)$, and $\int_0^{h_0} x^2\phi(x) dx = \mu_6(0)$. Then, there is $T_0 \in (0, T]$, such that there exists a unique solution $(h(t), b(t), c(t), v(y, t)) \in C^1[0, T_0] \times (C[0, T_0])^2 \times (C^{2,1}(Q_{T_0}) \cap C^{1,0}(\bar{Q}_{T_0}))$, $h(t) > 0$ for $t \in [0, T_0]$, of the inverse problem (7)–(9), (11), (12) and (35).

Proof. Following [18], let us introduce the notations

$$p(t) := h'(t), \quad w(y, t) := v_y(y, t). \quad (37)$$

Then, we can reduce the problem (7)–(9), (11), (12) and (35) to a system of integral equations for the unknowns $h(t)$, $p(t)$, $b(t)$, $c(t)$, $v(y, t)$ and $w(y, t)$, as follows.

First, let us denote by $G_1(y, t; \eta, \tau)$ the Green function of the Dirichlet boundary-value problem for the equation

$$\frac{\partial V}{\partial t}(y, t) = \frac{a(yh(t), t)}{h^2(t)} \frac{\partial^2 V}{\partial y^2}(y, t).$$

Then, $v(y, t)$ satisfying equations (7)–(9) can be represented in the form

$$v(y, t) = v_0(y, t) + \int_0^t \int_0^1 G_1(y, t; \eta, \tau) \left(\left(\frac{b(\tau) + \eta p(\tau)}{h(\tau)} \right) w(\eta, \tau) + c(\tau) v(\eta, \tau) \right) d\eta d\tau, \quad (38)$$

where $v_0(y, t)$ is given by, [11],

$$\begin{aligned} v_0(y, t) &= \int_0^1 G_1(y, t; \eta, 0) \phi(h_0 \eta) d\eta + \int_0^t \frac{\partial G_1}{\partial \eta}(y, t; 0, \tau) \frac{a(0, \tau)}{h^2(\tau)} \mu_1(\tau) d\tau \\ &\quad - \int_0^t \frac{\partial G_1}{\partial \eta}(y, t; 1, \tau) \frac{a(h(\tau), \tau)}{h^2(\tau)} \mu_2(\tau) d\tau + \int_0^t \int_0^1 G_1(y, t; \eta, \tau) f(\eta h(\tau), \tau) d\eta d\tau. \end{aligned} \quad (39)$$

Let us now rewrite the problem (7)–(9) for v into a new one for the partial derivative v_y which was denoted by w in (37). For this, we differentiate with respect to y equations (7) and (8), apply (7) at $y \in \{0, 1\}$ and use (9) to obtain

$$\begin{aligned} \frac{\partial w}{\partial t}(y, t) &= \frac{a(yh(t), t)}{h^2(t)} \frac{\partial^2 w}{\partial y^2}(y, t) + \left(\frac{a_x(yh(t), t) + b(t) + yh'(t)}{h(t)} \right) \frac{\partial w}{\partial y}(y, t) \\ &\quad + \left(\frac{h'(t)}{h(t)} + c(t) \right) w(y, t) + h(t) f_x(yh(t), t), \quad (y, t) \in Q_T, \end{aligned} \quad (40)$$

$$w(y, 0) = h_0 \phi'(h_0 y), \quad y \in [0, 1], \quad (41)$$

$$\frac{\partial w}{\partial y}(0, t) = \frac{h^2(t)}{a(0, t)} \left(\mu'_1(t) - \frac{b(t)}{h(t)} w(0, t) - c(t) \mu_1(t) - f(0, t) \right), \quad t \in [0, T], \quad (42)$$

$$\begin{aligned} \frac{\partial w}{\partial y}(1, t) &= \frac{h^2(t)}{a(h(t), t)} \left(\mu'_2(t) - \left(\frac{b(t) + h'(t)}{h(t)} \right) w(1, t) - c(t) \mu_2(t) - f(h(t), t) \right), \\ &\quad t \in [0, T]. \end{aligned} \quad (43)$$

Note that the boundary conditions (42) and (43) are of Neumann type. Denoting by $G_2(y, t; \eta, \tau)$ the Green function of the Neumann boundary-value problem for the equation

$$\frac{\partial W}{\partial t}(y, t) = \frac{a(yh(t), t)}{h^2(t)} \frac{\partial^2 W}{\partial y^2}(y, t) + \frac{a_x(yh(t), t)}{h(t)} \frac{\partial W}{\partial y}(y, t),$$

then, $w(y, t)$ satisfying equations (40)–(43), can be represented in the form

$$\begin{aligned} w(y, t) &= h_0 \int_0^1 G_2(y, t; \eta, 0) \phi'(h_0 \eta) d\eta \\ &\quad - \int_0^t G_2(y, t; 0, \tau) \left(\mu'_1(\tau) - \frac{b(\tau)}{h(\tau)} w(0, \tau) - c(\tau) \mu_1(\tau) - f(0, \tau) \right) d\tau \\ &\quad + \int_0^t G_2(y, t; 1, \tau) \left(\mu'_2(\tau) - \left(\frac{b(\tau) + h'(\tau)}{h(\tau)} \right) w(1, \tau) - c(\tau) \mu_2(\tau) - f(h(\tau), \tau) \right) d\tau \\ &\quad + \int_0^t \int_0^1 G_2(y, t; \eta, \tau) \left[\left(\frac{b(\tau) + \eta h'(\tau)}{h(\tau)} \right) \frac{\partial w}{\partial \eta}(\eta, \tau) + \left(\frac{h'(\tau)}{h(\tau)} + c(\tau) \right) w(\eta, \tau) \right. \\ &\quad \left. + h(\tau) f_x(\eta h(\tau), \tau) \right] d\eta d\tau. \end{aligned} \quad (44)$$

Integrating by parts in the expression

$$\int_0^t \int_0^1 G_2(y, t; \eta, \tau) \left(\frac{b(\tau) + \eta h'(\tau)}{h(\tau)} \right) \frac{\partial w}{\partial \eta}(\eta, \tau) d\eta d\tau$$

we represent (44) in the form

$$\begin{aligned} w(y, t) &= w_0(y, t) + \int_0^t \int_0^1 \left(G_2(y, t; \eta, \tau) c(\tau) \right. \\ &\quad \left. - G_{2\eta}(y, t; \eta, \tau) \left(\frac{b(\tau) + \eta h'(\tau)}{h(\tau)} \right) \right) w(\eta, \tau) d\eta d\tau, \end{aligned} \quad (45)$$

where $w_0(y, t)$ is expressed by

$$\begin{aligned}
w_0(y, t) = & h_0 \int_0^1 G_2(y, t; \eta, 0) \phi'(h_0 \eta) d\eta \\
& - \int_0^t G_2(y, t; 0, \tau) (\mu_1'(\tau) - c(\tau) \mu_1(\tau) - f(0, \tau)) d\tau \\
& + \int_0^t G_2(y, t; 1, \tau) (\mu_2'(\tau) - c(\tau) \mu_2(\tau) - f(h(\tau), \tau)) d\tau \\
& + \int_0^t \int_0^1 G_2(y, t; \eta, \tau) h(\tau) f_x(\eta h(\tau), \tau) d\eta d\tau.
\end{aligned} \tag{46}$$

From condition (11) we have

$$h(t) = \frac{\mu_4(t)}{\int_0^1 v(y, t) dy}, \quad t \in [0, T]. \tag{47}$$

Differentiating (11), (12) and (35) with respect to t and using (7) we obtain the following three equations in $b(t)$, $c(t)$ and $p(t)$:

$$\begin{aligned}
p(t) \mu_2(t) + b(t) (\mu_2(t) - \mu_1(t)) + c(t) \mu_4(t) = & \mu_4'(t) + \frac{1}{h(t)} (a(0, t) w(0, t) - a(h(t), t) w(1, t)) \\
& + \int_0^1 a_x(yh(t), t) w(y, t) dy - h(t) \int_0^1 f(yh(t), t) dy,
\end{aligned} \tag{48}$$

$$\begin{aligned}
p(t) h(t) \mu_2(t) + b(t) (h(t) \mu_2(t) - \mu_4(t)) + c(t) \mu_5(t) = & \mu_5'(t) - a(h(t), t) w(1, t) \\
& + \int_0^1 \left(yh(t) a_x(yh(t), t) + a(yh(t), t) \right) w(y, t) dy - h^2(t) \int_0^1 y f(yh(t), t) dy,
\end{aligned} \tag{49}$$

$$\begin{aligned}
p(t) h^2(t) \mu_2(t) + b(t) (h^2(t) \mu_2(t) - 2\mu_5(t)) + c(t) \mu_6(t) = & \mu_6'(t) - h(t) a(h(t), t) w(1, t) \\
& + h(t) \int_0^1 \left(2ya(yh(t), t) + y^2 h(t) a_x(yh(t), t) \right) w(y, t) dy - h^3(t) \int_0^1 y^2 f(yh(t), t) dy.
\end{aligned} \tag{50}$$

By solving the system of equations (48)–(50) in $p(t)$, $b(t)$ and $c(t)$ using the *Mathematica 7.0* symbolic computation package we obtain

$$\begin{aligned}
p(t) = & \left\{ h^4(t)(int2 - int6)\mu_2(t)\mu_4(t) + h^3(t)[int4\mu_2(t)\mu_5(t) \right. \\
& - int2(\mu_4^2(t) + (\mu_2(t) - \mu_1(t))\mu_5(t))] \\
& - \frac{(aw0 - aw1)(2\mu_5^2(t) - \mu_4(t)\mu_6(t))}{h(t)} - h^2(t)[int1\mu_2(t)\mu_4(t) - int5\mu_2(t)\mu_4(t) \\
& + int3\mu_2(t)\mu_5(t) - 2int6\mu_4(t)\mu_5(t) + int6\mu_1(t)\mu_6(t) + int4\mu_2(t)\mu_6(t) \\
& - int6\mu_2(t)\mu_6(t) + \mu_2(t)\mu_5(t)\mu_4'(t) - \mu_2(t)\mu_4(t)\mu_5'(t)] \\
& + h(t)[aw0\mu_2(t)\mu_5(t) - 2int4\mu_5^2(t) + int1(\mu_4^2(t) - \mu_1(t)\mu_5(t) + \mu_2(t)\mu_5(t)) \\
& - aw1(\mu_4^2(t) - \mu_1(t)\mu_5(t) + 2\mu_2(t)\mu_5(t)) + int3\mu_2(t)\mu_6(t) + int4\mu_4(t)\mu_6(t) \\
& + \mu_2(t)\mu_6(t)\mu_4'(t) - \mu_2(t)\mu_4(t)\mu_6'(t)] + 2aw1\mu_4(t)\mu_5(t) - 2int5\mu_4(t)\mu_5(t) \\
& + 2int3\mu_5^2(t) - aw1\mu_1(t)\mu_6(t) + int5\mu_1(t)\mu_6(t) - aw0\mu_2(t)\mu_6(t) + 2aw1\mu_2(t)\mu_6(t) \\
& - int5\mu_2(t)\mu_6(t) - int3\mu_4(t)\mu_6(t) + 2\mu_5^2(t)\mu_4'(t) - \mu_4(t)\mu_6(t)\mu_4'(t) - 2\mu_4(t)\mu_5(t)\mu_5'(t) \\
& + \mu_1(t)\mu_6(t)\mu_5'(t) - \mu_2(t)\mu_6(t)\mu_5'(t) + \mu_4^2(t)\mu_6'(t) - \mu_1(t)\mu_5(t)\mu_6'(t) \\
& \left. + \mu_2(t)\mu_5(t)\mu_6'(t) \right\} / (\mu_2(t)D_2(t)), \tag{51}
\end{aligned}$$

$$\begin{aligned}
b(t) = & \left(h^4(t)(int6 - int2)\mu_4(t) + h^3(t)(int2 - int4)\mu_5(t) + aw0\mu_6(t) - 2aw1\mu_6(t) \right. \\
& + int5\mu_6(t) + \mu_6(t)\mu_5'(t) + h^2(t)[int1\mu_4(t) - int5\mu_4(t) + int3\mu_5(t) + int4\mu_6(t) \\
& - int6\mu_6(t) + \mu_5(t)\mu_4'(t) - \mu_4(t)\mu_5'(t)] - \mu_5(t)\mu_6'(t) - h(t)[aw0\mu_5(t) - 2aw1\mu_5(t) \\
& \left. + int1\mu_5(t) + int3\mu_6(t) + \mu_6(t)\mu_4'(t) - \mu_4(t)\mu_6'(t) \right) / D_2(t), \tag{52}
\end{aligned}$$

$$\begin{aligned}
c(t) = & \left(h^4(t)(int6 - int2)\mu_1(t) + h^3(t)(int2 - int4)\mu_4(t) + 2aw0\mu_5(t) - 4aw1\mu_5(t) \right. \\
& + 2int5\mu_5(t) + 2\mu_5(t)\mu_5'(t) + h^2(t)[int1\mu_1(t) - int5\mu_1(t) + int3\mu_4(t) + 2int4\mu_5(t) \\
& - 2int6\mu_5(t) + \mu_4(t)\mu_4'(t) - \mu_1(t)\mu_5'(t)] - \mu_4(t)\mu_6'(t) - h(t)[aw0\mu_4(t) - 2aw1\mu_4(t) \\
& \left. + int1\mu_4(t) + 2int3\mu_5(t) + 2\mu_5(t)\mu_4'(t) - \mu_1(t)\mu_6'(t) \right) / D_2(t), \tag{53}
\end{aligned}$$

where $awi = a(ih(t), t)w(i, t)$ for $i = 0, 1$,

$$int1 = \int_0^1 (2ya(yh(t), t) + y^2h(t)a_x(yh(t), t))w(y, t)dy,$$

$$int2 = \int_0^1 y^2f(yh(t), t)dy, \quad int3 = \int_0^1 a_x(yh(t), t)w(y, t)dy,$$

$$int4 = \int_0^1 f(yh(t), t)dy, \quad int5 = \int_0^1 (a(yh(t), t) + yh(t)a_x(yh(t), t))w(y, t)dy,$$

$$int6 = \int_0^1 yf(yh(t), t)dy, \text{ and}$$

$$\begin{aligned}
D_2(t) := & h^2(t)(\mu_4^2(t) - \mu_1(t)\mu_5(t)) + h(t)(\mu_1(t)\mu_6(t) - 2\mu_4(t)\mu_5(t)) \\
& + 2\mu_5^2(t) - \mu_4(t)\mu_6(t), \quad t \in [0, T]. \tag{54}
\end{aligned}$$

Condition (36) is equivalent to $D_2(0) \neq 0$, and since all the functions in (54) are continuous in $[0, T]$ we obtain that $D_2(t) \neq 0$ in an upper neighborhood $[0, T_1]$ of $t = 0$, where $T_1 \in (0, T]$.

So, at least locally in this neighborhood of $t = 0$ the denominator in (51)-(53) do not vanish and hence, these expressions for $p(t)$, $b(t)$ and $c(t)$ are well-defined.

To summarise, equations (51)-(53) express the unknowns $p(t)$, $b(t)$ and $c(t)$ in terms of $h(t)$ and $w(y, t)$, and we join these with equations (38), (45) and (47).

Next, we establish local (in time) estimates for the unknowns $v(y, t)$, $h(t)$, $w(y, t)$, $p(t)$, $b(t)$ and $c(t)$. From (39), the properties of the Green function G_1 and since $f \geq 0$, $\mu_1 > 0$ and $\mu_2 > 0$, we have

$$\begin{aligned} v_0(y, t) &\geq \min\left\{\min_{y \in [0,1]} \phi(h_0 y), \min_{t \in [0,T]} \mu_1(t), \min_{t \in [0,T]} \mu_2(t)\right\} \left(\int_0^1 G_1(y, t; \eta, 0) d\eta\right) \\ &+ \int_0^t \frac{\partial G_1}{\partial \eta}(y, t; 0, \tau) \frac{a(0, \tau)}{h^2(\tau)} d\tau - \int_0^t \frac{\partial G_1}{\partial \eta}(y, t; 1, \tau) \frac{a(h(\tau), \tau)}{h^2(\tau)} d\tau \\ &= \min\left\{\min_{y \in [0,1]} \phi(h_0 y), \min_{t \in [0,T]} \mu_1(t), \min_{t \in [0,T]} \mu_2(t)\right\} =: M_0 > 0, \quad (y, t) \in \overline{Q}_T, \end{aligned} \quad (55)$$

where, in the last identity, use has been made of the Green formula for the function identically equal to 1. Similarly, we have

$$v_0(y, t) \leq \max\left\{\max_{y \in [0,1]} \phi(h_0 y), \max_{t \in [0,T]} \mu_1(t), \max_{t \in [0,T]} \mu_2(t), f_0 T\right\} =: M_1 < \infty, \quad (y, t) \in \overline{Q}_T. \quad (56)$$

Since the second-term in the right hand side of (38) is a continuous function which is zero at $t = 0$, its absolute value can be made arbitrary small (say $\leq \frac{1}{2}M_0$) in a sufficiently small neighbourhood $[0, T_2]$ with $T_2 \in (0, T]$. Then from this, (38), (55) and (56) we obtain the local estimates for $v(y, t)$ in the form,

$$\frac{1}{2}M_0 \leq v(y, t) \leq M_1 + \frac{1}{2}M_0, \quad (y, t) \in \overline{Q}_{T_2}. \quad (57)$$

Applying (47) we also obtain the local estimates for $h(t)$ in the form

$$0 < H_0 := \frac{\min_{t \in [0,T]} \mu_4(t)}{\frac{1}{2}M_0 + M_1} \leq h(t) \leq H_1 < \infty, \quad t \in [0, T_2], \quad (58)$$

where H_1 is given by (33).

To summarise, expressions (57) and (58) give the local estimates for $v(y, t)$ and $h(t)$. In order to estimate the remaining unknowns let us define $W(t) := \max_{y \in [0,1]} |w(y, t)|$ and observe that from (51)–(53), using (58), we obtain

$$\begin{aligned} |p(t)| &\leq C_1 + C_2 W(t), & |b(t)| &\leq C_3 + C_4 W(t), \\ |c(t)| &\leq C_5 + C_6 W(t), & t &\in [0, T_2], \end{aligned} \quad (59)$$

where, from now on in the proof, C_i , $i = 1, 2, \dots$ denote generic positive constants. Using the estimates of the Green function G_2 , see [14],

$$|G_2(y, t; \eta, \tau)| \leq \frac{C}{\sqrt{t - \tau}}, \quad \int_0^1 |G_{2\eta}(y, t; \eta, \tau)| d\eta \leq \frac{C}{\sqrt{t - \tau}}, \quad (60)$$

for some positive constant C , and applying (59), from (45) and (46), we find that

$$\begin{aligned}
W(t) &\leq C_7 + C_8 \int_0^t \frac{(|b(\tau)| + |p(\tau)|)W(\tau) + |c(\tau)|}{\sqrt{t-\tau}} d\tau \\
&\leq C_9 + C_{10} \int_0^t \frac{W(\tau) + W^2(\tau)}{\sqrt{t-\tau}} d\tau \leq C_{11} + C_{12} \int_0^t \frac{W^2(\tau)}{\sqrt{t-\tau}} d\tau, \quad t \in [0, T_2].
\end{aligned} \tag{61}$$

Square both sides of (61) and use the Cauchy-Bunyakowski inequality to obtain

$$W^2(t) \leq C_{13} + C_{14} \int_0^t \frac{W^4(\tau)}{\sqrt{t-\tau}} d\tau, \quad t \in [0, T_2]. \tag{62}$$

Replacing t by σ , we multiply (62) by $\frac{1}{\sqrt{t-\sigma}}$ and integrate from 0 to t to obtain

$$\int_0^t \frac{W^2(\sigma)}{\sqrt{t-\sigma}} d\sigma \leq C_{13} \sqrt{T_2} + C_{14} \int_0^t \frac{d\sigma}{\sqrt{t-\sigma}} \int_0^\sigma \frac{W^4(\tau)}{\sqrt{\sigma-\tau}} d\tau, \quad t \in [0, T_2]. \tag{63}$$

Changing the order of integration in the second term of the right-hand side of (63), we get

$$\int_0^t \frac{W^2(\sigma)}{\sqrt{t-\sigma}} d\sigma \leq C_{13} \sqrt{T_2} + C_{15} \int_0^t W^4(\tau) d\tau, \quad t \in [0, T_2]. \tag{64}$$

Using (64) in (61) we obtain

$$W(t) \leq C_{16} + C_{17} \int_0^t W^4(\tau) d\tau, \quad t \in [0, T_2]. \tag{65}$$

This inequality has been solved in [11, p.126] to obtain the local estimate

$$W(t) \leq M_2 < \infty, \quad t \in [0, T_3], \tag{66}$$

in the neighbourhood of $t = 0$, where $T_3 \in (0, T]$. Finally, with the aid of (66), from (59) we find the local estimates

$$|p(t)| \leq M_3, \quad |b(t)| \leq M_3, \quad |c(t)| \leq M_3, \quad t \in [0, T_3]. \tag{67}$$

Now the Schauder fixed-point theorem for completely continuous operators can be applied to establish the local existence of solution. The remainder of the proof based on the Volterra integral equations of the second kind to establish the uniqueness of solution is similar to the proof from [18] and therefore, is omitted.

Remarks.

(i) In the computations we need the values of $b(0)$ and $c(0)$. These are given by equations (20), (21) or, (23), (24) or, (52), (53) applied at $t = 0$.

(ii) As in Section 2, one can further elaborate on the expression (54) giving the determinant of the system of equations (51)-(53), as follows. Substitute in (54) the expressions for $\mu_4(t)$, $\mu_5(t)$ and $\mu_6(t)$ by the integral moments (11), (12) and (35) to obtain

$$D_2(t) = h^4(t) \left[\mu_1(t) \int_0^1 y(y-1)v(y,t)dy - \int_0^1 v(y,t)dy \int_0^1 y^2v(y,t)dy \right. \\ \left. + \left(\int_0^1 yv(y,t)dy \right)^2 + \left(\int_0^1 (1-y)v(y,t)dy \right)^2 \right]. \quad (68)$$

Transform (68), as follows:

$$\frac{D_2(t)}{h^4(t)} = \int_0^1 v(y,t)dy \int_0^1 y(y-1)v(y,t)dy + \int_0^1 (v(0,t) - v(y,t))dy \int_0^1 y(y-1)v(y,t)dy \\ - \int_0^1 v(y,t)dy \int_0^1 y^2v(y,t)dy + \left(\int_0^1 yv(y,t)dy \right)^2 + \left(\int_0^1 (1-y)v(y,t)dy \right)^2.$$

Changing one of the variables in integrals, we obtain

$$\frac{D_2(t)}{h^4(t)} = \int_0^1 (v(0,t) - v(\xi,t))d\xi \int_0^1 y(y-1)v(y,t)dy \\ + \int_0^1 [y(y-1) - y^2 + \xi y + (1-\xi)(1-y)]v(\xi,t)v(y,t)d\xi dy. \\ = - \int_0^1 y(y-1)v(y,t)dy \int_0^1 d\xi \int_0^\xi v_\xi(\xi,t)d\xi \\ + \int_0^1 \int_0^1 (1-\xi)(1-2y)v(\xi,t)v(y,t)d\xi dy. \quad (69)$$

Now using the identity

$$\int_0^1 (1-2y)v(y,t)dy = \int_0^{1/2} (1-2y)(v(y,t) - v(1-y,t))dy \\ = - \int_0^{1/2} (1-2y)dy \int_y^{1-y} v_\xi(\xi,t)d\xi$$

into (69) yields

$$\frac{D_2(t)}{h^4(t)} = \int_0^1 y(1-y)v(y,t)dy \int_0^1 (1-\xi)v_\xi(\xi,t)d\xi \\ - \int_0^1 (1-\xi)v(\xi,t)d\xi \int_0^{1/2} (1-2y)dy \int_y^{1-y} v_\xi(\xi,t)d\xi.$$

Changing the order of the integration in the last integral, after some calculus we obtain

$$\frac{D_2(t)}{h^4(t)} = \int_0^1 y(1-y)v(y,t)dy \int_0^1 (1-\xi)v_\xi(\xi,t)d\xi \\ - \int_0^1 (1-y)v(y,t)dy \int_0^1 \xi(1-\xi)v_\xi(\xi,t)d\xi \\ = \int_0^1 \int_0^1 v(y,t)v_\xi(\xi,t)(1-\xi)(1-y)(y-\xi)d\xi dy.$$

Decomposing the integration in the unit square onto integrations in the domains $y < \xi$ and $y > \xi$, we obtain

$$\begin{aligned} \frac{D_2(t)}{h^4(t)} &= \int_0^1 dy \int_0^y (1-\xi)(1-y)(y-\xi) \left(v(y,t)v_\xi(\xi,t) - v_y(y,t)v(\xi,t) \right) d\xi \\ &= \int_0^1 dy \int_0^y (1-\xi)(1-y)(y-\xi)v(y,t)v(\xi,t) \left(\frac{v_\xi(\xi,t)}{v(\xi,t)} - \frac{v_y(y,t)}{v(y,t)} \right) d\xi. \end{aligned} \quad (70)$$

Again, from the fact that $\mu_1 > 0$, $\mu_2 > 0$, $\phi > 0$, $f \geq 0$ we obtain from the minimum principle that $v > 0$. Moreover, if the function $v_\xi(\xi,t)/v(\xi,t)$ is strictly monotone, then from (70) it follows that $D_2(t) \neq 0$. This condition can be ensured locally if $\phi \in C^2[0, h_0]$ and $\ln(\phi)$ is strictly convex or concave function.

(iii) In [18], stronger assumptions than (36) were used, namely that

$$\mu_6(t)\mu_1(t) - 2\mu_4(t)\mu_5(t) > 0, \quad \mu_4^2(t) - \mu_1(t)\mu_5(t) > 0, \quad t \in [0, T]. \quad (71)$$

and

$$\begin{aligned} &\mu_4(t)\mu_6(t) - 2\mu_5^2(t) - H_1(\mu_1(t)\mu_6(t) - 2\mu_4(t)\mu_5(t)) \\ &- H_1^2(\mu_4^2(t) - \mu_1(t)\mu_5(t)) > 0, \quad t \in [0, T], \end{aligned} \quad (72)$$

where H_1 is given by (33). However, it is not obvious whether one can find an example for which these conditions hold. Instead, the simpler assumption $D_2(0) \neq 0$ given by (36) is sufficient for the local existence and uniqueness of solution.

3 Solution of direct problem

In this section, we consider the direct initial boundary value problem (1)–(3), where $h(t)$, $b(t)$, $c(t)$, $a(x, t)$, $f(x, t)$, $\phi(x)$, and $\mu_i(t)$, $i = 1, 2$, are known and the solution $u(x, t)$ is to be determined, additionally to the quantities of interest $\mu_i(t)$, $i = 3, 6$. To achieve this, we use the Crank-Nicolson finite-difference scheme [17], based on subdividing the solution domain $Q_T = (0, 1) \times (0, T)$ into M and N subintervals of equal step lengths Δy and Δt , where $\Delta y = 1/M$ and $\Delta t = T/N$, respectively. At the node (i, j) we denote $v_{i,j} := v(y_i, t_j)$, where $y_i = i\Delta y$, $t_j = j\Delta t$, $a_{i,j} := a(y_i, t_j)$, $h_j := h(t_j)$, $b_j := b(t_j)$, $c_j := c(t_j)$ and $f_{i,j} := f(y_i, t_j)$ for $i = \overline{0, M}$ and $j = \overline{0, N}$.

Once the solution $v_{i,j}$ for $i = \overline{0, M}$, $j = \overline{0, N}$ has been determined accurately, the data (10)–(12) and (35) can be calculated using the following finite-difference approximation formula and trapezoidal rule for integrals:

$$\mu_3(t_j) = \frac{h_j - h_{j-1}}{\Delta t} - \frac{4v_{M-1,j} - v_{M-2,j} - 3v_{M,j}}{2(\Delta y)h_j}, \quad j = \overline{1, N}, \quad (73)$$

$$\mu_{k+3}(t_j) = \frac{h_j^k}{2N} \left(y_0^{k-1}v_{0,j} + y_M^{k-1}v_{M,j} + 2 \sum_{i=1}^{M-1} y_i^{k-1}v_{i,j} \right), \quad j = \overline{1, N}, \quad k = 1, 2, 3. \quad (74)$$

4 Numerical approach to the inverse problems

In the inverse problems stated in Section 2, we wish to obtain simultaneously stable reconstructions of the two unknown coefficients $b(t)$ and $c(t)$, together with the free boundary

$h(t)$ and the transformed temperature $v(y, t)$, satisfying equations (7)–(12) or, (7)–(9), (11), (12) and (35), by minimizing the Tikhonov regularized nonlinear objective function

$$F(\underline{h}, \underline{b}, \underline{c}) = \sum_{j=1}^N \left[h'_j + \frac{v_y(1, t_j)}{h_j} - \mu_3(t_j) \right]^2 + \sum_{j=1}^N \left[h_j \int_0^1 v(y, t_j) dy - \mu_4(t_j) \right]^2 \\ + \sum_{j=1}^N \left[h_j^2 \int_0^1 yv(y, t_j) dy - \mu_5(t_j) \right]^2 + \beta_1 \sum_{j=1}^N h_j^2 + \beta_2 \sum_{j=1}^N b_j^2 + \beta_3 \sum_{j=1}^N c_j^2, \quad (75)$$

or,

$$F_1(\underline{h}, \underline{b}, \underline{c}) = \sum_{j=1}^N \left[h_j \int_0^1 v(y, t_j) dy - \mu_4(t_j) \right]^2 + \sum_{j=1}^N \left[h_j^2 \int_0^1 yv(y, t_j) dy - \mu_5(t_j) \right]^2 \\ + \sum_{j=1}^N \left[h_j^3 \int_0^1 y^2v(y, t_j) dy - \mu_6(t_j) \right]^2 + \beta_1 \sum_{j=1}^N h_j^2 + \beta_2 \sum_{j=1}^N b_j^2 + \beta_3 \sum_{j=1}^N c_j^2, \quad (76)$$

respectively. The unregularized case, i.e., $\beta_i = 0$ for $i = 1, 2, 3$, yields the ordinary non-linear least-squares method which usually produces unstable solutions for noisy data. The minimization of F or (F_1) subject to the physical constraint for the free boundary $\underline{h} > \underline{0}$ is performed using the MATLAB optimization toolbox routine *lsqnonlin*. This routine attempts to find a minimum of a sum of squares, starting from an initial guess, subject to constraints. We take bounds for the positive quantity $h(t)$ say, we seek it in the interval $(10^{-10}, 10^2)$ and the bounds for the quantities $b(t)$ and $c(t)$ say, we seek them in the interval $(-10^2, 10^2)$. We also take the parameters of the routine as follows:

- Number of variables $M = N$.
- Maximum number of iterations = $10 \times (\text{number of variables})$.
- Maximum number of objective function evaluations = $10^5 \times (\text{number of variables})$.
- Solution and object function tolerances = 10^{-15} .

In (75), we approximate the derivative of $h(t)$ as

$$h'_j := h'(t_j) \approx \frac{h(t_j) - h(t_{j-1})}{\Delta t} = \frac{h_j - h_{j-1}}{\Delta t}, \quad j = \overline{1, N}. \quad (77)$$

Condition (4) represents a Stefan condition of melting between a solid and a fluid and, in general, μ_3 is taken to be zero (or is assumed to be prescribed exactly). Therefore, practically the experimental measurement errors are likely to be only in the heat moments (5), (6) and (34). In order to model these errors, we replace $\mu_{k+3}(t_j)$, $k = 1, 2, 3$, in equations (11), (12) and (34) by $\mu_{k+3}^{\epsilon k}(t_j)$, as

$$\mu_{k+3}^{\epsilon k}(t_j) = \mu_{k+3}(t_j) + \epsilon k_j, \quad k = 1, 2, 3, \quad j = \overline{1, N}, \quad (78)$$

where ϵk_j are random variables generated from a Gaussian normal distribution with mean zero and standard deviation σ_k , given by

$$\sigma_k = p \times \max_{t \in [0, T]} |\mu_{k+3}(t)|, \quad k = 1, 2, 3, \quad (79)$$

where p represents the percentage of noise.

5 Numerical results and discussion

In this section, we present a couple of typical test examples to illustrate the accuracy and stability of the numerical scheme based on the FDM with $M = N = 40$ combined with minimization of the nonlinear objective function (75) or (76), as described in Section 4. To assess the accuracy of the approximate solutions, let us introduce the root mean squares error (*rmse*) defined as

$$rmse(h) = \sqrt{\frac{T}{N} \sum_{j=1}^N (h_{numerical}(t_j) - h_{exact}(t_j))^2}, \quad (80)$$

$$rmse(b) = \sqrt{\frac{T}{N} \sum_{j=1}^N (b_{numerical}(t_j) - b_{exact}(t_j))^2}, \quad (81)$$

$$rmse(c) = \sqrt{\frac{T}{N} \sum_{j=1}^N (c_{numerical}(t_j) - c_{exact}(t_j))^2}. \quad (82)$$

5.1 Example 1

We consider the first inverse problem (1)–(6) with unknown coefficients $h(t)$, $b(t)$ and $c(t)$, and the following input data:

$$\begin{aligned} a(x, t) &= \frac{(1+x)(1+t)}{2}, \quad \phi(x) = \frac{1}{1+x}, \quad \mu_1(t) = e^{3t}, \quad \mu_2(t) = \frac{e^{3t}}{2+t}, \\ \mu_3(t) &= 1 - \frac{e^{3t}}{(2+t)^2}, \quad \mu_4(t) = e^{3t} \ln(2+t), \quad \mu_5(t) = e^{3t}(1+t - \ln(2+t)), \\ f(x, t) &= \frac{e^{3t}(2-t)}{1+x}, \quad h_0 = 1, \quad T = 1. \end{aligned}$$

One can remark that conditions of Theorem 1 are satisfied hence, the local uniqueness of this solution is guaranteed. Furthermore, one can observe that the function (22) given by

$$D_1(t) = e^{6t} \left(\ln^2(2+t) - \frac{(1+t)^2}{2+t} \right), \quad t \in [0, 1], \quad (83)$$

is negative and hence it does not vanish on $[0, 1]$. Thus, expressions (23) and (24) for $b(t)$ and $c(t)$, respectively, are well-defined over the whole time interval $[0, 1]$. Remark also that $(\ln \phi(x))'' = 1/(1+x)^2$ is positive and hence it does not vanish on $[0, 1]$.

With the above data the analytical solution of the inverse problem (1)–(6) is given by

$$h(t) = 1+t, \quad b(t) = 1+t, \quad c(t) = 1+t, \quad (84)$$

$$u(x, t) = \frac{e^{3t}}{1+x}. \quad (85)$$

We also have that the analytical solution of the transformed inverse problem (7)–(12) is given by equation (84) and

$$v(y, t) = u(yh(t), t) = \frac{e^{3t}}{1+y+yt}. \quad (86)$$

The initial guesses for the vectors \underline{h} , \underline{b} and \underline{c} are taken as $\underline{1}$, namely,

$$h_j^0 = b_j^0 = c_j^0 = 1, \quad j = \overline{1, N}. \quad (87)$$

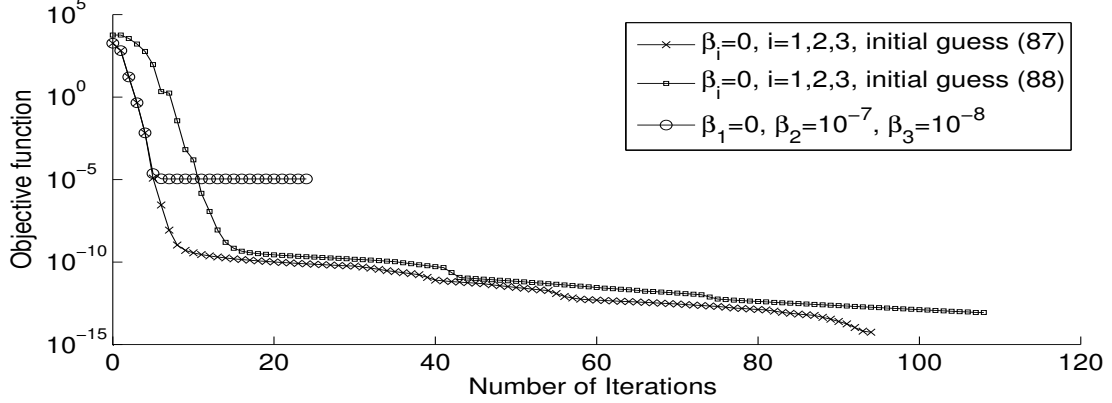


Figure 1: The objective function (75) without noise for Example 1.

We consider first the case where there is no noise in the input data (10)–(12), i.e. $p = 0$ in (79). The objective function (75), as a function of the number of iterations is presented in Figure 1. From this figure it can be seen that a monotonic decreasing convergence is rapidly achieved in a few iterations. The objective function (75) decreases rapidly and takes a stationary value of $O(10^{-15})$ in about 95 iterations when we do not employ any regularization, i.e. $\beta_i = 0$, $i = 1, 2, 3$. In order to investigate the robustness of the nonlinear iterative routine *lsqnonlin* employed for minimizing the objective function (75), in Figure 1 we also include the convergence history for a different than (87) initial guess for the unknowns \underline{h} , \underline{b} and \underline{c} namely,

$$h_j^0 = b_j^0 = c_j^0 = 1 - \frac{t_j}{2}, \quad j = \overline{1, N}. \quad (88)$$

As expected, from this farther initial guess (88) to the exact solution (84) than (87) it takes a slighter larger number of iterations (108 instead of 95), but the minimization of the objective function (75) converges to similar very small minimum values which are of $O(10^{-15})$ to $O(10^{-14})$. This means that the routine used is robust by being quite insensitive to the initial guess for the unknowns. In the remaining of this subsection and the next subsection 5.2, figures are illustrated only for the initial guess (87). Although not illustrated, we report that similar numerical results have been obtained for the other initial guess (88).

The corresponding numerical results for the unknowns $h(t)$, $b(t)$ and $c(t)$ are presented in Figure 2. From this figure it can be noticed that a stable and very accurate retrieval for the free boundary $h(t)$ is obtained with a small $rmse(h) = 1.7E - 4$. Consequently, there is no need to regularize h and therefore, in what follows, we take $\beta_1 = 0$ in (75). The numerical reconstructions for $b(t)$ and $c(t)$ are stable, but with less accurate values of $rmse(b) = 0.0472$ and $rmse(c) = 0.0260$, respectively. However, when we add a little regularization with $\beta_2 = 10^{-7}$, $\beta_3 = 10^{-8}$ to (75) we obtain a faster convergence in about 25 iterations to reach a stationary value of $O(10^{-5})$, see Figure 1, and even more stable and accurate results for $b(t)$ and $c(t)$ with $rmse$ values decreasing to $rmse(b) = 0.0394$ and $rmse(c) = 0.0213$, respectively, see Figure 2.

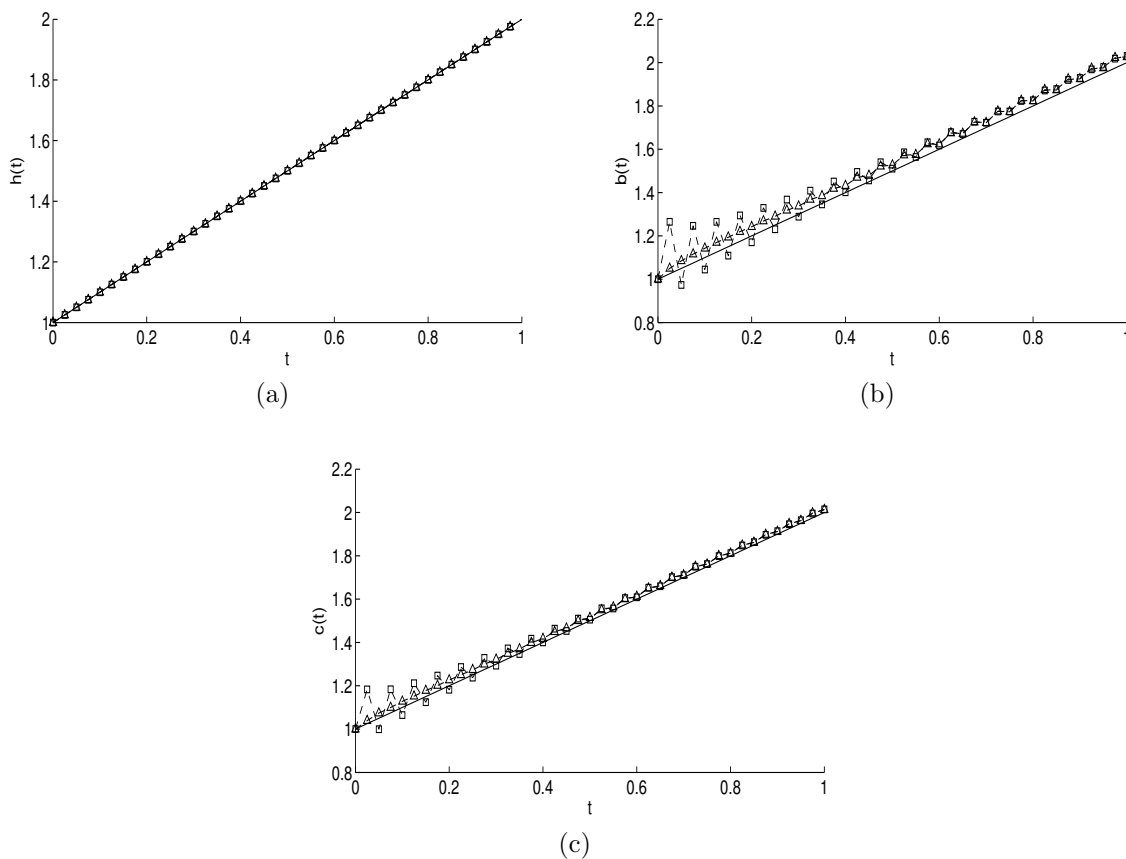


Figure 2: The exact (—) and numerical solutions without regularization ($-\square-$), and with regularization parameters $\beta_1 = 0$, $\beta_2 = 10^{-7}$ and $\beta_3 = 10^{-8}$ ($-\triangle-$) for: (a) the free boundary $h(t)$, (b) the coefficient $b(t)$, and (c) the coefficient $c(t)$, without noise for Example 1.

Next, in order to investigate the stability of the numerical solution we add some small percentage $p = 0.1\%$ of noise to the input data (11) and (12), as in (78) for $k = 1, 2$. We have also investigated higher amounts of noise p , but the results obtained were less accurate hence, they are not presented. However, similar qualitative conclusions, regarding achieving stability through regularization, maintain. Details regarding the number of iterations, number of function evaluations, value of the objective function (75) at the final iteration, the *rmse* values (80)–(82) and the computational time taken for running the iterative minimization routine *lsqnonlin* are summarised in Table 1. One can notice that it takes almost one day to run the program without regularization.

The objective function (75), as a function of the number of iterations, is plotted in Figure 3. From this figure it can be seen that in the absence of regularization, see the graph for $\beta_i = 0$, $i = 1, 2, 3$, a slow convergence is recorded and, in fact, the process of minimization of the routine *lsqnonlin* is stopped when the prescribed maximum number of 400 iterations is reached. The corresponding numerical results for the unknown coefficients are presented in Figure 4. From Figure 4(a) it can be seen that stable and accurate numerical results are obtained for the free boundary $h(t)$. However, from Figures 4(b) and 4(c) one can observe that unstable (highly oscillatory and unbounded) and very inaccurate solutions for $b(t)$ and $c(t)$ are obtained. This is expected since the problem under investigation is ill-posed and small errors in the measurement data (11) and (12) lead to a drastic amount of error in the output coefficients $b(t)$ and $c(t)$. Therefore, regularization should be applied to restore

the stability of the solution in the components $b(t)$ and $c(t)$. Since in Figure 4(a) the free boundary has been obtained accurately, we fix $\beta_1 = 0$ and we only take β_2 and β_3 as positive regularization parameters in (75). These regularization parameters have been chosen by trial and error, and some numerical results obtained from a couple of choices are given in Table 1, and Figures 3 and 5. Justifying more rigorously the choice of multiple regularization parameters in the nonlinear Tikhonov regularization method is very challenging and will be the object of future numerical investigations. At this stage, we only mention the idea of extending to the nonlinear case some possible strategies of multi-parameter selection for the linear Tikhonov regularization suggested in [3]. From Figure 3 it can be noticed that a rapid convergence in less than 30 iterations is achieved for each selection of regularization parameters. Furthermore, from Table 1 it can be seen that the computational time is reduced from 1 day to less than an hour by the inclusion of regularization in (75).

Table 1: Number of iterations, number of function evaluations, value of the objective function (75) at final iteration, $rmse$ values (80)-(82) and the computational time, for $p = 0.1\%$ noise for Example 1.

$\beta_1 = 0$	$\beta_2 = \beta_3 = 0$	$\beta_2 = \beta_3 = 10^{-4}$	$\beta_2 = \beta_3 = 10^{-3}$
No. of iterations	401	23	28
No. of function evaluations	49446	2976	3596
Value of objective function (75) at final iteration	0.0026	0.0345	0.1412
$rmse(h)$	0.0108	0.0026	0.0040
$rmse(b)$	105.34	1.1044	1.0787
$rmse(c)$	61.838	0.8184	0.6558
Computational time	23 hours	40 min	45 min

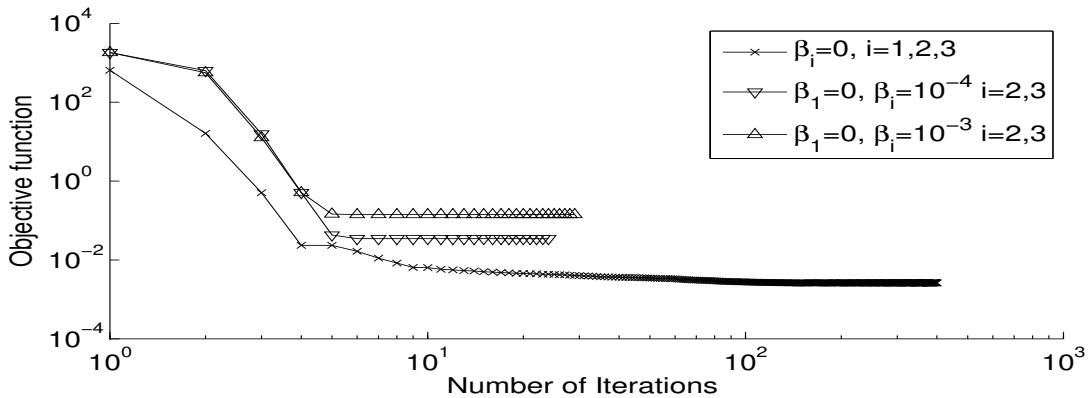


Figure 3: The objective function (75) for $p = 0.1\%$ noise for Example 1.

The corresponding numerical reconstructions for the unknown free boundary $h(t)$ and the coefficients $b(t)$ and $c(t)$ are presented in Figures 5(a)-(c), respectively. By comparing Figures 4(b) and 4(c) with 5(b) and 5(c) one can immediately observe the dramatic improvement in stability and accuracy which is achieved through the inclusion of regularization in the objective function (75).

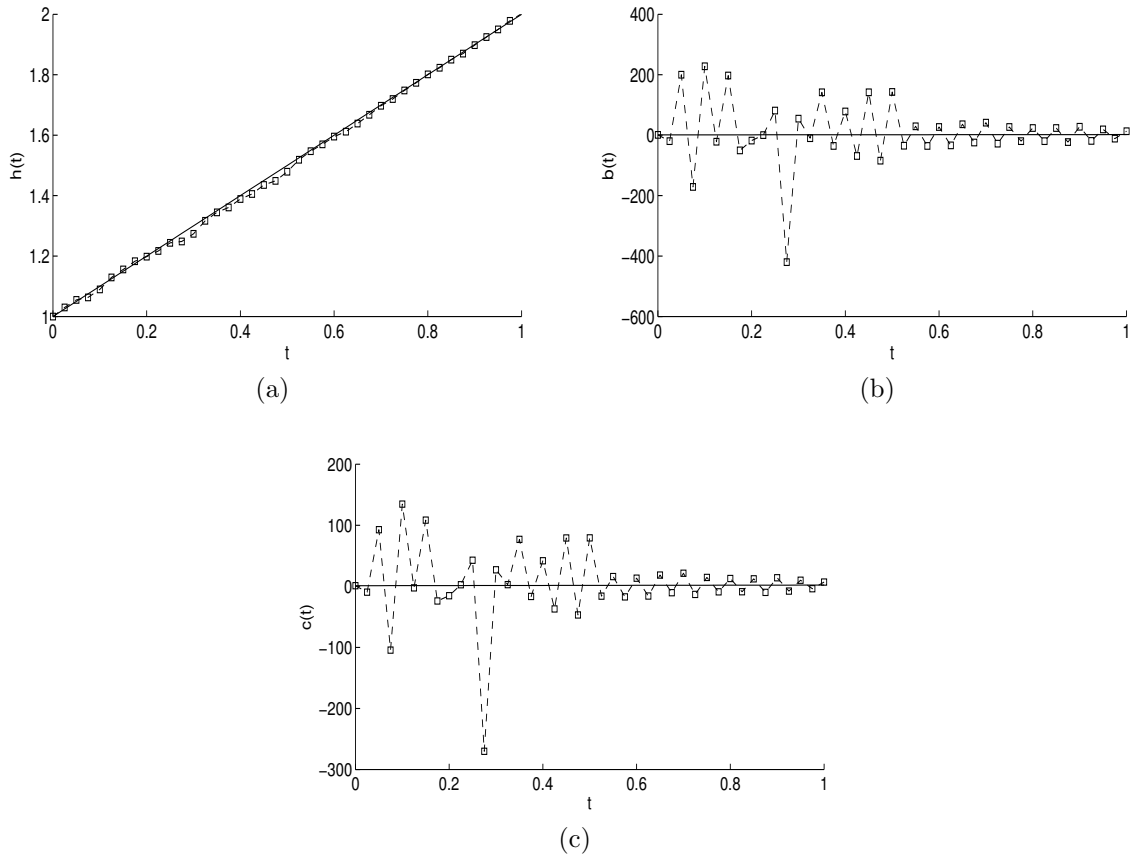


Figure 4: The exact (—) and numerical (—□—) solutions for: (a) the free boundary $h(t)$, (b) the coefficient $b(t)$, and (c) the coefficient $c(t)$, with $p = 0.1\%$ noise and no regularization for Example 1.

5.2 Example 2

We consider now the second inverse problem (1)–(3), (5), (6) and (34) with unknown coefficients $h(t)$, $b(t)$ and $c(t)$, with the same input data as in Example 1 of Subsection 5.1, but in which the Stefan condition data $\mu_3(t)$ given by equation (4) is replaced by the third-order heat moment $\mu_6(t)$ given by equation (35) as

$$\mu_6(t) = \frac{e^{3t}}{2}(t^2 - 1 + 2 \ln(2 + t)), \quad t \in [0, 1].$$

One can remark that conditions of Theorem 2 are satisfied and therefore, the local existence of a unique solution is guaranteed. Furthermore, one can observe that the function (54) given by

$$D_2(t) = - (1/2)e^{6t} \left((t-1)(1+t)^2 + (7+10t+3t^2) \ln(2+t) - 2(2+t)^2 \ln^2(2+t) \right), \quad t \in [0, 1], \quad (89)$$

is negative and hence it does not vanish on $[0, 1]$. Hence, expressions (52) and (53) for $b(t)$ and $c(t)$, respectively, are well-defined over the whole time interval $[0, 1]$. The analytical

solution is the same as that given by equations (84) and (85). All the computational details are the same as for Example 1.

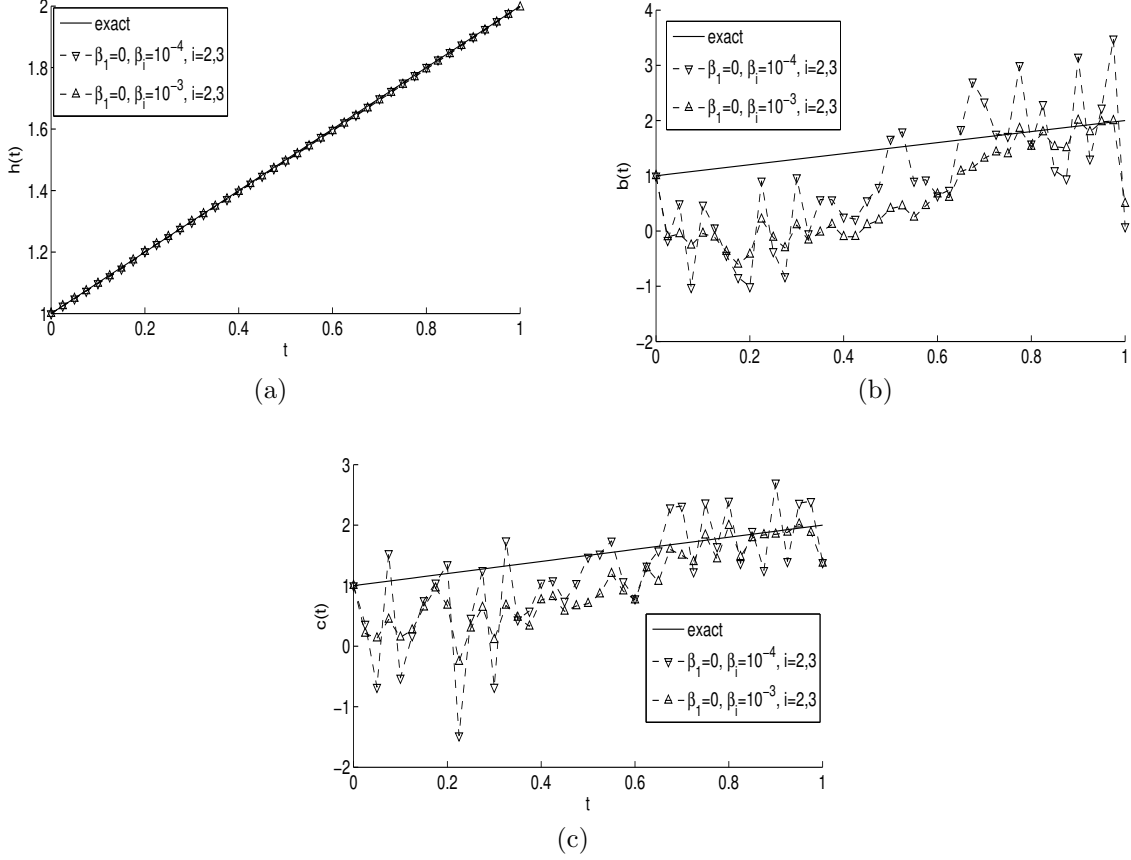


Figure 5: The exact and numerical solutions for: (a) the free boundary $h(t)$, (b) the coefficient $b(t)$, and (c) the coefficient $c(t)$, with $p = 0.1\%$ noise and regularization for Example 1.

As we did in Example 1, we start with the case of exact input data (11), (12) and (35), i.e. $p = 0$ in (79). The objective function (76), as a function of the number of iterations is displayed in Figure 6. From this figure it can be noticed that a monotonic convergence is rapidly achieved (in the early few iterations) and then turn to a steady slow convergence. The objective function (76) decreases and takes stationary values of $O(10^{-11})$ and $O(10^{-6})$ in about 401 and 112 iterations for $\beta_i = 0$, $i = 1, 2, 3$, and $\beta_1 = 0$, $\beta_2 = \beta_3 = 10^{-8}$, respectively. The numerical results for the unknown coefficients are illustrated in Figure 7. From this figure it can be noticed that, as in Example 1, a stable and very accurate recovery for the free boundary $h(t)$ is obtained with a small $rmse(h) = 0.001$. With no regularization, the numerical results for $b(t)$ and $c(t)$ are quite unstable and inaccurate with $rmse$ values of 0.5962 and 0.4279, respectively. However, when we apply the regularization with $\beta_1 = 0$, and $\beta_2 = \beta_3 = 10^{-8}$ to (76) we obtain more stable and accurate reconstructions for $b(t)$ and $c(t)$ with $rmse$ values decreasing to 0.2908 and 0.1838, respectively.

Next, we consider the case of noisy input data (11), (12) and (35) and perturb them with $p = 0.01\%$ as in (78). Remark that in Example 2 we include noise in all the input data μ_4 , μ_5 and μ_6 , whilst in Example 1 noise was included only in μ_4 and μ_5 . Therefore, in Example 2 we take a smaller percentage of noise than in Example 1. In addition, the investigation of the inversion of noisy data performed in this subsection, when compared

with that of Example 1, indicates that the second inverse problem (1)–(3), (5), (6) and (34) is more ill-posed than the first inverse problem (1)–(6). The case when no regularization is included, i.e. $\beta_i = 0$ for $i = 1, 2, 3$, is omitted since a similar unstable behaviour to Example 1 shown in Figures 4(b) and 4(c) was obtained. The regularized objective function (76) with $\beta_1 = 0$, $\beta_2 = \beta_3 = 10^{-6}$ shown in Figure 6 decreases rapidly and takes a stationary value of $O(10^{-3})$ in 63 iterations. With this selection of regularization parameters, the unknown coefficients are plotted in Figure 7 using the dashed line style (- - -). The coefficients are reconstructed with reasonable accuracy having the *rmse* values of 0.0022, 0.9498 and 0.6781 for $h(t)$, $b(t)$ and $c(t)$, respectively.

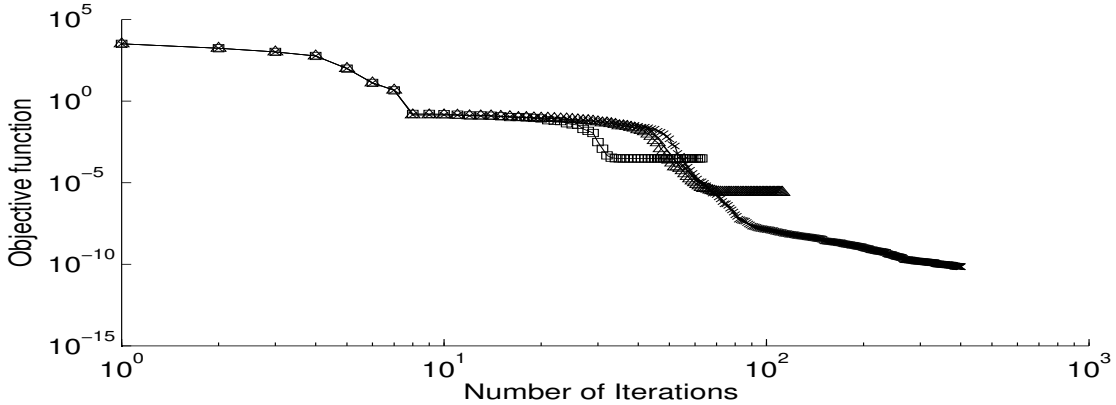


Figure 6: The objective function (76) with no regularization (-x-) and with regularization parameters $\beta_1 = 0$, $\beta_2 = \beta_3 = 10^{-8}$ (- Δ -), without noise for Example 2. We also include with (- \square -) the results for $p = 0.01\%$ noise, with regularization parameters $\beta_1 = 0$, $\beta_2 = \beta_3 = 10^{-6}$.

The next section investigates inverse problems similar to those of Sections 2, 4 and 5, but in which the time-dependent thermal conductivity is an additional unknown.

6 Triple coefficient extension

Consider the one-dimensional time-dependent heat equation

$$\frac{\partial u}{\partial t}(x, t) = a(t) \frac{\partial^2 u}{\partial x^2}(x, t) + b(t) \frac{\partial u}{\partial x}(x, t) + c(t)u(x, t) + f(x, t), \quad (x, t) \in \Omega \quad (90)$$

for the unknown temperature $u(x, t)$ with unknown free smooth boundary $x = h(t) > 0$ and time-dependent coefficients $a(t) > 0$, $b(t)$ and $c(t)$. The initial and Dirichlet boundary conditions are (2) and (3), respectively, and the over-determination conditions are (4)–(6), together with the heat flux specification at $x = 0$, namely,

$$-a(t)u_x(0, t) = \tilde{\mu}_3(t), \quad t \in [0, T]. \quad (91)$$

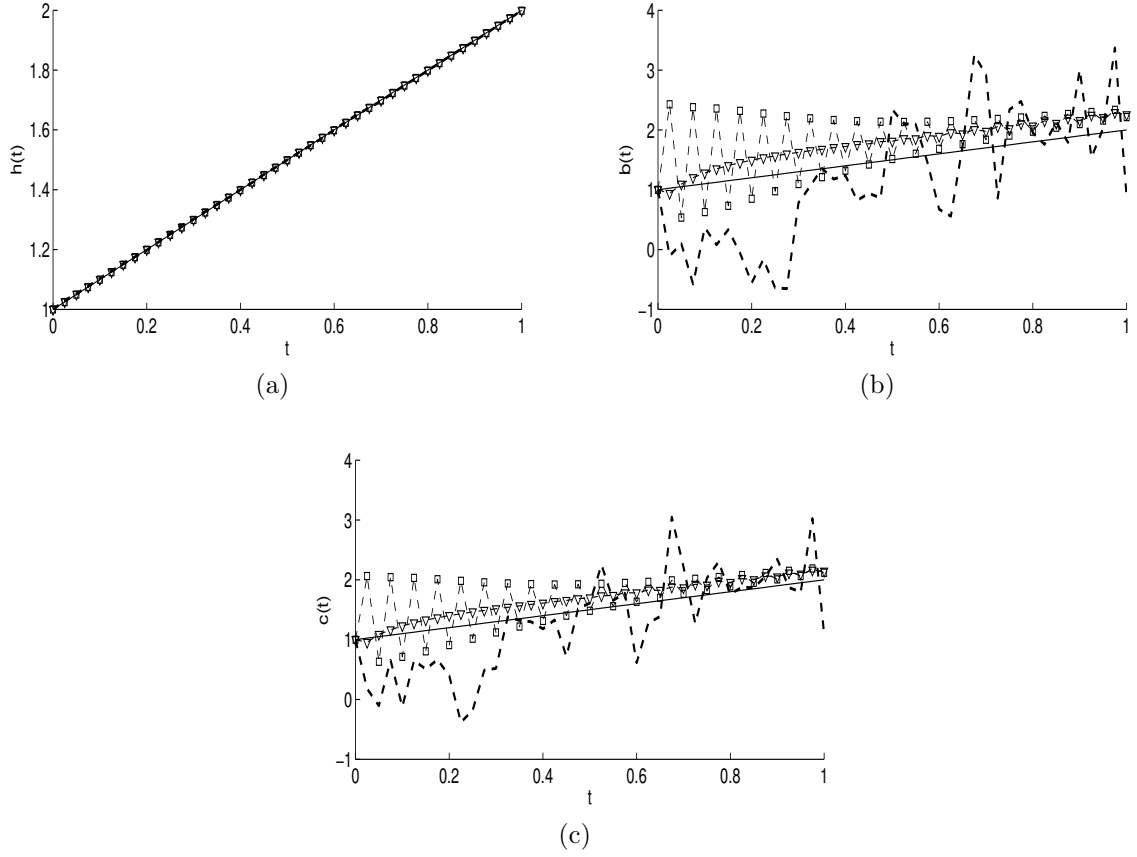


Figure 7: The exact (—) and numerical solutions with no regularization ($\square\square\square$), and with regularization parameters $\beta_1 = 0$, $\beta_2 = \beta_3 = 10^{-8}$ ($\triangle\triangle\triangle$) without noise for Example 2. We also include with (- - -) the numerical results for $p = 0.01\%$ noise with regularization parameters $\beta_1 = 0$, $\beta_2 = \beta_3 = 10^{-6}$ for: (a) the free boundary $h(t)$, (b) the coefficient $b(t)$, and (c) the coefficient $c(t)$.

As in Section 2, by performing the change of variable $y = x/h(t)$ we reduce the problem (2)–(6), (90) and (91) to the inverse problem for the unknowns $h(t)$, $a(t)$, $b(t)$, $c(t)$ and $v(y, t) := u(yh(t), t)$ given by:

$$\frac{\partial v}{\partial t}(y, t) = \frac{a(t)}{h^2(t)} \frac{\partial^2 v}{\partial y^2}(y, t) + \frac{b(t) + yh'(t)}{h(t)} \frac{\partial v}{\partial y}(y, t) + c(t)v(y, t) + f(yh(t), t), \quad (y, t) \in Q_T, \quad (92)$$

equations (8)–(12) and

$$-\frac{a(t)v_y(0, t)}{h(t)} = \tilde{\mu}_3(t), \quad t \in [0, T]. \quad (93)$$

A slightly corrected version of the theorem proved in [19] ensures the unique solvability (locally in time) for the inverse problem (8)–(12), (92) and (93).

Theorem 3. *Suppose that:*

$0 \leq f \in C^{1,0}([0, \infty) \times [0, T])$, $0 < \mu_i \in C^1[0, T]$ for $i = 1, 2, 4, 5$, $\mu_3 \in C[0, T]$, $0 > \tilde{\mu}_3 \in C[0, T]$, $0 < \phi \in C^2[0, h_0]$, $\phi' > 0$,

$$(\ln \phi)'' \neq 0, \quad (94)$$

the compatibility conditions of the zero order:

$\phi(0) = \mu_1(0)$, $\phi(h_0) = \mu_2(0)$, $\int_0^{h_0} \phi(x)dx = \mu_4(0)$, $\int_0^{h_0} x\phi(x)dx = \mu_5(0)$,
and of the first-order:

$$\left. \begin{aligned} \mu'_1(0) &= a(0)\phi''(0) + b(0)\phi'(0) + c(0)\phi(0) + f(0,0), \\ \mu'_2(0) &= a(0)\phi''(h_0) + b(0)\phi'(h_0) + c(0)\phi(h_0) + f(h_0,0), \end{aligned} \right\} \quad (95)$$

are satisfied. Then, there is $T_0 \in (0, T]$, such that there exists a unique solution $(h(t), a(t), b(t), c(t), v(y, t)) \in C^1[0, T_0] \times (C[0, T_0])^3 \times C^{2,1}(\overline{Q}_{T_0})$, $h(t) > 0$, $a(t) > 0$ for $t \in [0, T_0]$, of the inverse problem (8)–(12), (92) and (93).

Remark. We can obtain the values of $a(0)$, $b(0)$ and $c(0)$ directly from equations (93) and (95). First, from (93) applied at $t = 0$ we have

$$a(0) = -\frac{\tilde{\mu}_3(0)}{\phi'(0)}. \quad (96)$$

Then, introducing (96) into (95) and solving the resulting system of equations for $b(0)$ and $c(0)$ we obtain

$$b(0) = \frac{\phi(h_0) \left(\mu'_1(0) + \frac{\tilde{\mu}_3(0)\phi''(0)}{\phi'(0)} - f(0,0) \right) - \phi(0) \left(\mu'_2(0) + \frac{\tilde{\mu}_3(0)\phi''(h_0)}{\phi'(0)} - f(h_0,0) \right)}{\phi(0)\phi(h_0) \left(\frac{\phi'(0)}{\phi(0)} - \frac{\phi'(h_0)}{\phi(h_0)} \right)}, \quad (97)$$

$$c(0) = \frac{\phi'(0) \left(\mu'_2(0) + \frac{\tilde{\mu}_3(0)\phi''(h_0)}{\phi'(0)} - f(h_0,0) \right) - \phi'(h_0) \left(\mu'_1(0) + \frac{\tilde{\mu}_3(0)\phi''(0)}{\phi'(0)} - f(0,0) \right)}{\phi(0)\phi(h_0) \left(\frac{\phi'(0)}{\phi(0)} - \frac{\phi'(h_0)}{\phi(h_0)} \right)}. \quad (98)$$

One can easily remark that the conditions on ϕ given in Theorem 3 ensure that expressions (97) and (98) are well-defined. In particular, condition (94) implies that the function ϕ'/ϕ is strictly monotone.

6.1 Another related inverse problem formulation

It was point out in [12] that the Stefan condition (4), or (10), may be replaced by the second-order moment measurement (34), or (35), respectively. Then we have the following local existence and uniqueness theorem, see [12] with appropriate corrections.

Theorem 4. *Let the assumptions of Theorem 3 be satisfied, except for the condition on μ_3 being replaced by the condition $0 < \mu_6 \in C^1[0, T]$. Then, there exists $T_0 \in (0, T]$, such that there exists a unique solution $(h(t), a(t), b(t), c(t), v(y, t)) \in C^1[0, T_0] \times (C[0, T_0])^3 \times C^{2,1}(\overline{Q}_{T_0})$, $h(t) > 0$, $a(t) > 0$ for $t \in [0, T_0]$, of the inverse problem (8), (9), (11), (12), (92) and (93).*

6.2 Numerical implementation, results and discussion

The solution of the direct problem is based on the same FDM described in Section 3 with the simplification that the thermal conductivity coefficient a depends now on t only. For the

inverse problems under investigation in Section 6 we minimize the functionals

$$\begin{aligned}
\tilde{F}(\underline{h}, \underline{a}, \underline{b}, \underline{c}) &= \sum_{j=1}^N \left[\frac{a_j v_y(0, t_j)}{h_j} + \tilde{\mu}_3(t_j) \right]^2 + \sum_{j=1}^N \left[h'_j + \frac{v_y(1, t_j)}{h_j} - \mu_3(t_j) \right]^2 \\
&+ \sum_{j=1}^N \left[h_j \int_0^1 v(y, t_j) dy - \mu_4(t_j) \right]^2 + \sum_{j=1}^N \left[h_j^2 \int_0^1 y^2 v(y, t_j) dy - \mu_5(t_j) \right]^2 \\
&+ \beta_1 \sum_{j=1}^N h_j^2 + \beta_2 \sum_{j=1}^N a_j^2 + \beta_3 \sum_{j=1}^N b_j^2 + \beta_4 \sum_{j=1}^N c_j^2,
\end{aligned} \tag{99}$$

and

$$\begin{aligned}
\tilde{F}_1(\underline{h}, \underline{a}, \underline{b}, \underline{c}) &= \sum_{j=1}^N \left[\frac{a_j v_y(0, t_j)}{h_j} + \tilde{\mu}_3(t_j) \right]^2 + \sum_{j=1}^N \left[h_j \int_0^1 v(y, t_j) dy - \mu_4(t_j) \right]^2 \\
&+ \sum_{j=1}^N \left[h_j^2 \int_0^1 y v(y, t_j) dy - \mu_5(t_j) \right]^2 + \sum_{j=1}^N \left[h_j^3 \int_0^1 y^2 v(y, t_j) dy - \mu_6(t_j) \right]^2 \\
&+ \beta_1 \sum_{j=1}^N h_j^2 + \beta_2 \sum_{j=1}^N a_j^2 + \beta_3 \sum_{j=1}^N b_j^2 + \beta_4 \sum_{j=1}^N c_j^2.
\end{aligned} \tag{100}$$

The minimization of \tilde{F} and \tilde{F}_1 subject to the physical constraints $\underline{h} > \underline{0}$ and $\underline{a} > \underline{0}$ are performed using the MATLAB optimization toolbox routine *lsqnonlin*, as described in Section 4. We also add noise in the heat flux (93), as described at the end of Section 4.

6.2.1 Example 3

We consider first the inverse problem (2)–(6), (90) and (91) with unknown coefficients $h(t)$, $a(t)$, $b(t)$ and $c(t)$, and solve this problem with the following input data:

$$\begin{aligned}
\phi(x) = u(x, 0) &= (1+x)^2, \quad \mu_1(t) = u(0, t) = 1+t, \quad \mu_2(t) = u(h(t), t) = (1+t)(2+t)^2, \\
\tilde{\mu}_3(t) &= -a(t)u_x(0, t) = -2(1+t)^2, \quad \mu_3(t) = h'(t) + u_x(h(t), t) = 1 + 2(1+t)(2+t),
\end{aligned}$$

$$\mu_4(t) = \int_0^{h(t)} u(x, t) dx = \frac{1}{3}(1+t)^2(7+5t+t^2),$$

$$\mu_5(t) = \int_0^{h(t)} x u(x, t) dx = \frac{1}{12}(1+t)^3(17+14t+3t^2)$$

$$f(x, t) = 2 + 5t + 4t^2 + 6x + 12tx + 8t^2x + 2x^2 + 3tx^2 + 2t^2x^2, \quad h_0 = 1, \quad T = 1.$$

One can remark that the conditions of Theorem 3 are satisfied and hence, the local unique solvability of the inverse problem holds. With the data above, the analytical solution is given by

$$h(t) = 1+t, \quad a(t) = 1+t, \quad b(t) = -1-2t, \quad c(t) = -1-2t, \tag{101}$$

$$u(x, t) = (1+t)(1+x)^2. \tag{102}$$

Then, (101) and

$$v(y, t) = u(yh(t), t) = (1+t)(1+y+yt)^2, \tag{103}$$

is the analytical solution of the problem (8)–(12), (92) and (93).

The initial guess for the vectors \underline{h} , \underline{a} , \underline{b} and \underline{c} are taken as $\underline{1}$, $\underline{1}$, $\underline{-1}$ and $\underline{-1}$, respectively.

We start the numerical discussion with the case of exact data, i.e. $p = 0$ in (79). The objective function (99), as a function of the number of iterations, is shown in Figure 8. From this figure it can be seen that a monotonic convergence is achieved in 50 iterations if no regularization is applied. The unregularized objective function (99) decreases rapidly in the first 10 iterations and then steadily reaches a stationary low value of $O(10^{-16})$. The numerical results for the unknowns coefficients $h(t)$, $c(t)$, $b(t)$ and $c(t)$ are represented in Figures 9(a)–(d) by the (–x–) lines. From these figures it can be observed that we obtain accurate and stable reconstructions for free boundary $h(t)$ and the thermal conductivity $a(t)$, whilst for the coefficients $b(t)$ and $c(t)$ some very slight instabilities appear. Consequently, we do not need to regularize $h(t)$ and $a(t)$ and therefore, we are take $\beta_1 = \beta_2 = 0$ in (99) and apply the Tikhonov regularization method with some small regularization parameters $\beta_3 = \beta_4 = 10^{-5}$. The accurate and stable numerically obtained results are shown in Figures 9(a)–(d) by the (–□–) line. The regularized objective function (99) for this case is also plotted in Figure 8 and a rapid monotone convergence is obtained in 26 iterations. A summary of all details is presented in Table 2, where the $rmse(a)$ is defined, similarly as in (80)–(82), as

$$rmse(a) = \sqrt{\frac{T}{N} \sum_{j=1}^N (a_{numerical}(t_j) - a_{exact}(t_j))^2}. \quad (104)$$

Table 2: Number of iterations, number of function evaluations, value of the objective function (99) at final iteration, $rmse$ values (80)–(82) and (104), and the computational time, without noise for Example 3.

$\beta_1 = \beta_2 = 0$	$\beta_3 = \beta_4 = 0$	$\beta_3 = \beta_4 = 10^{-5}$
No. of iterations	50	26
No. of function evaluations	8415	4455
Value of objective function (99) at final iteration	6.2E-16	0.0035
$rmse(h)$	3.3E-4	3.3E-4
$rmse(a)$	0.0021	0.0021
$rmse(b)$	0.0333	0.0207
$rmse(c)$	0.0335	0.0149
Computational time	90 min	50 min

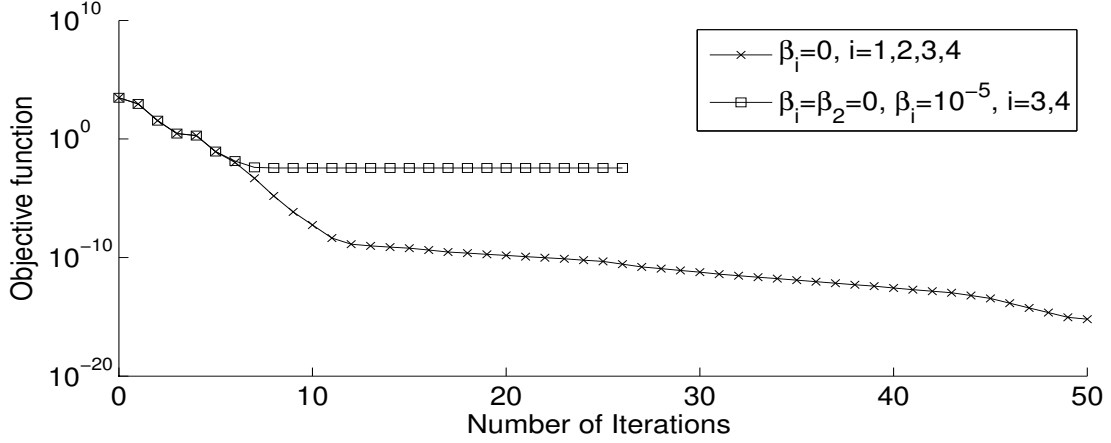


Figure 8: The objective function (99) without noise for Example 3.

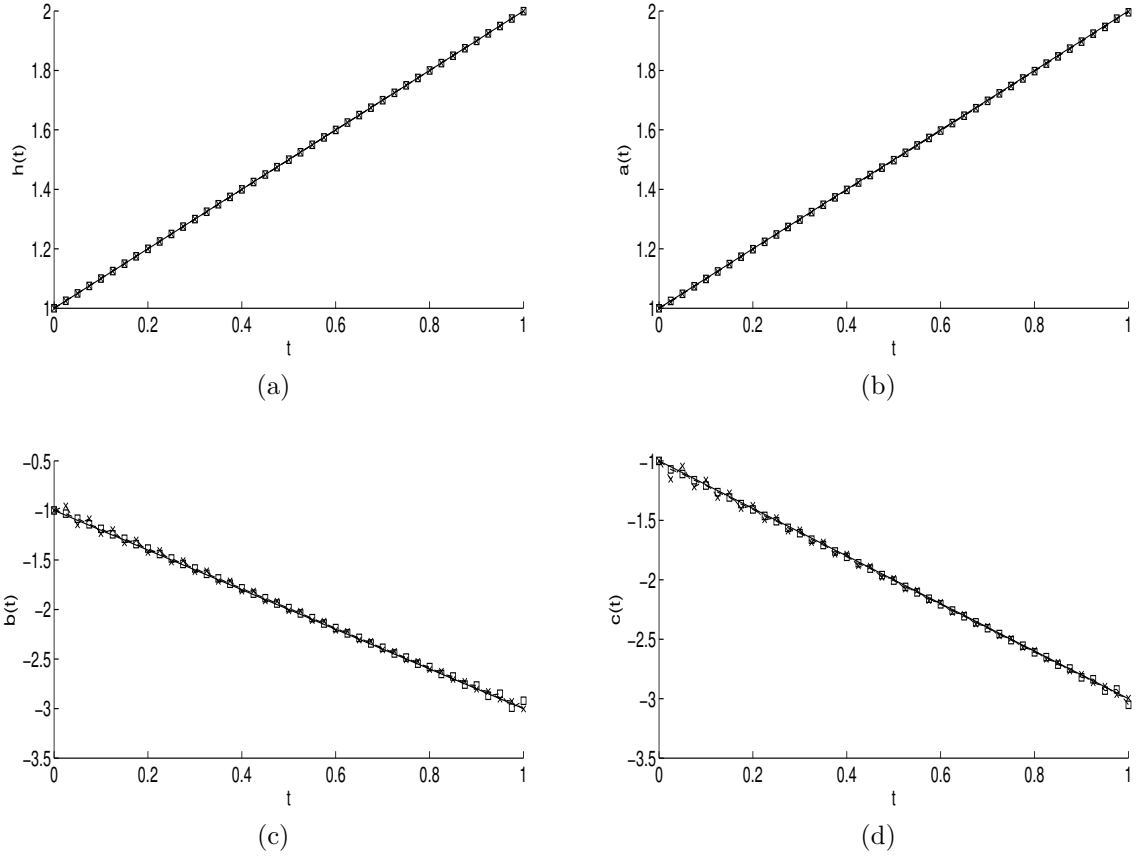


Figure 9: The exact (—) and numerical solutions (—x—) without regularization, and (—□—) with regularization parameters $\beta_1 = \beta_2 = 0$, and $\beta_3 = \beta_4 = 10^{-5}$ for: (a) the free boundary $h(t)$, (b) the coefficient $a(t)$, (c) the coefficient $b(t)$, and (d) the coefficient $c(t)$, without noise for Example 3.

Next, we investigate the stability of the numerical solution with respect to some small percentage $p = 0.1\%$ of noise included in the input data $\tilde{\mu}_3(t)$, $\mu_4(t)$ and $\mu_5(t)$. The objective function (99), as a function of the number of iterations in the case of no regularization employed is plotted in Figure 10. From this figure it can be noticed that a monotonic decreasing convergence is achieved and the minimization process stops when the allowed

tolerance is reached. On the other hand, the numerical solutions for the unknown coefficients plotted in Figure 11 are oscillatory and highly unstable except for the free boundary $h(t)$ which is accurate and stable. There is also some slight instability manifested in Figure 11(b) in estimating the coefficient $a(t)$, but the magnitude of these oscillations is significantly much smaller than the highly unbounded and unstable behaviour shown in Figures 11(c) and 11(d) illustrating the estimation of the unregularized coefficients $b(t)$ and $c(t)$, respectively. As a result, we can take $\beta_1 = \beta_2 = 0$ and then minimize (99) with various regularization parameters $\beta_3 = \beta_4 \in \{10^{-4}, 10^{-3}, 10^{-2}\}$. Figure 12 shows the rapid monotonic decreasing convergence of the regularized objective function, as the number of iterations increases. The corresponding numerical results for the unknown time-dependent coefficients are shown in Figures 13. A summary of the computational details, as well as the *rmse* errors are included in Table 3. Overall, by comparing Figures 11 and 13 it can be observed some remarkable stability restored through the inclusion of regularization. It is also interesting to remark that although we take $\beta_2 = 0$ and hence we do not penalise the coefficient $a(t)$ in (99), some of the regularization of the other two coefficients $b(t)$ and $c(t)$ is transferred to the former unregularized coefficient $a(t)$, compare Figures 11(b) and 13(b).

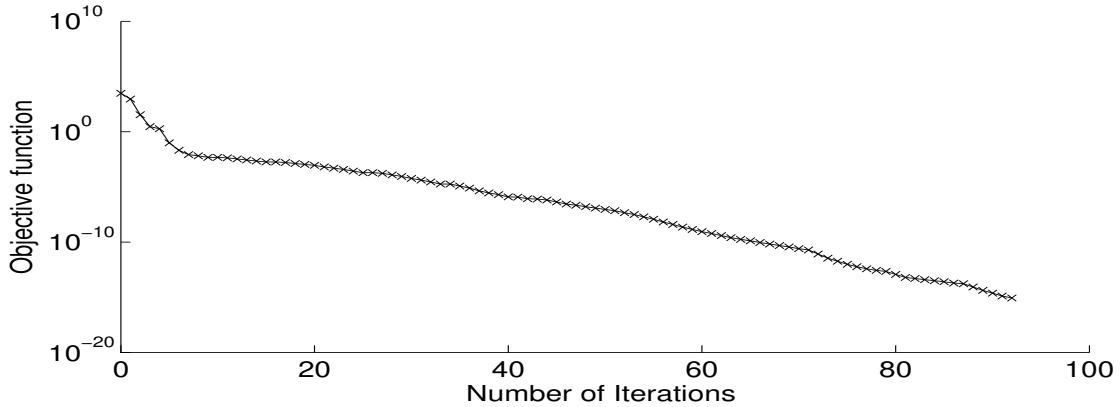


Figure 10: The objective function (99) with $p = 0.1\%$ noise and no regularization for Example 3.

Table 3: Number of iterations, number of function evaluations, value of the objective function (99) at final iteration, *rmse* values (80)-(82) and (104), and the computational time, for $p = 0.1\%$ noise for Example 3.

$\beta_1 = \beta_2 = 0$	$\beta_3 = \beta_4 = 0$	$\beta_3 = \beta_4 = 10^{-4}$	$\beta_3 = \beta_4 = 10^{-3}$	$\beta_3 = \beta_4 = 10^{-2}$
No. of iterations	92	27	25	30
No. of function evaluations	15354	4620	4290	5115
Value of objective function (99) at final iteration	8.4E-16	0.0449	0.3660	3.5102
<i>rmse</i> (h)	0.0043	0.0026	0.0022	0.0032
<i>rmse</i> (a)	0.2508	0.0487	0.0253	0.0398
<i>rmse</i> (b)	8.3489	0.5420	0.1991	0.2276
<i>rmse</i> (c)	7.8212	0.4354	0.1563	0.1646
Computational time	168 min	52 min	48 min	58 min

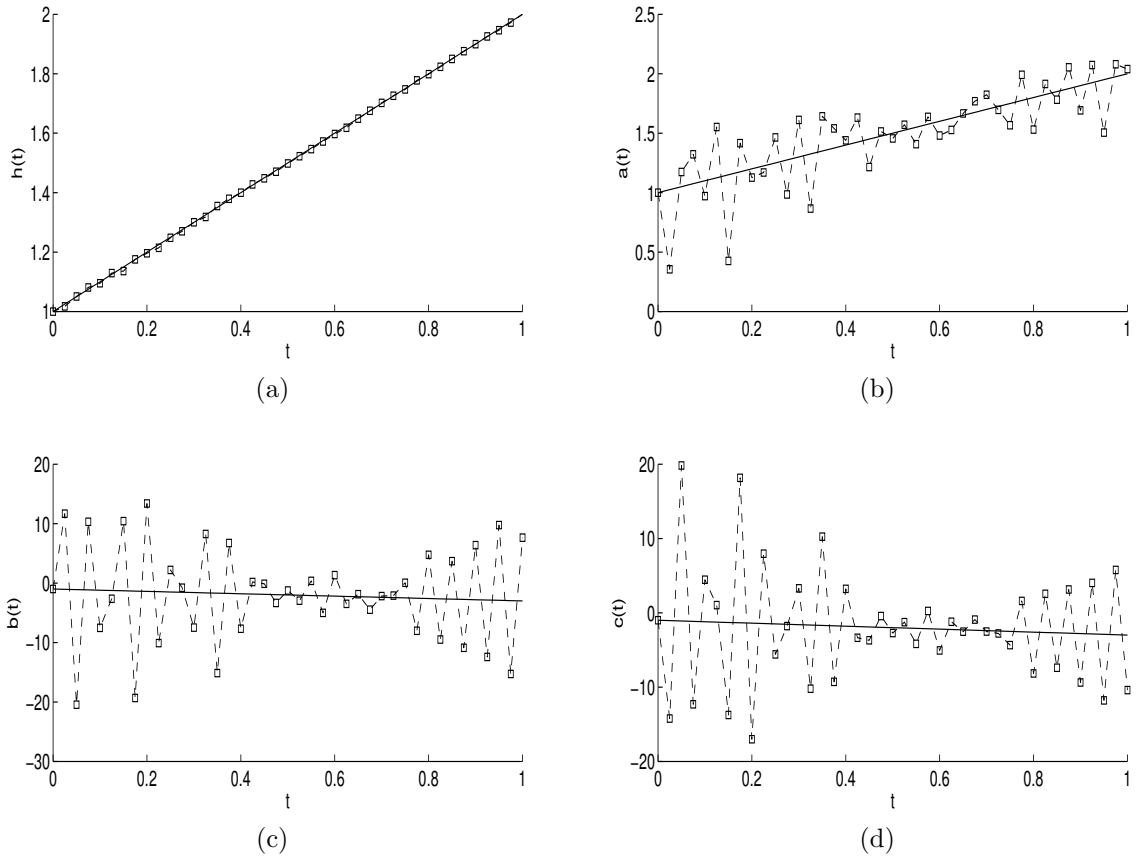


Figure 11: The exact (—) and numerical solution (—□—) for: (a) the free boundary $h(t)$, (b) the coefficient $a(t)$, (c) the coefficient $b(t)$, and (d) the coefficient $c(t)$, with $p = 0.1\%$ noise and no regularization for Example 3.

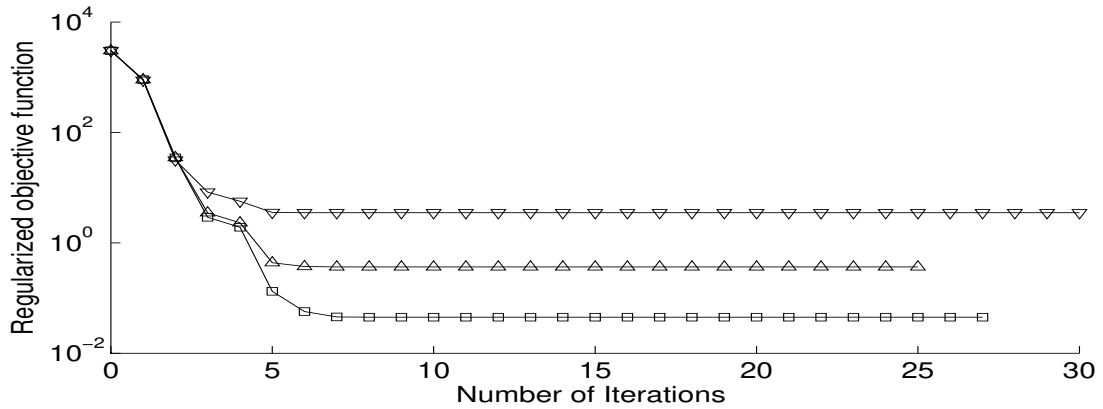


Figure 12: The regularized objective function (99), with regularization parameters $\beta_1 = \beta_2 = 0$, and $\beta_i = 10^{-4}$ (—□—), $\beta_i = 10^{-3}$ (—▽—), $\beta_i = 10^{-2}$ (—△—), $i = 3, 4$, with $p = 0.1\%$ noise for Example 3.

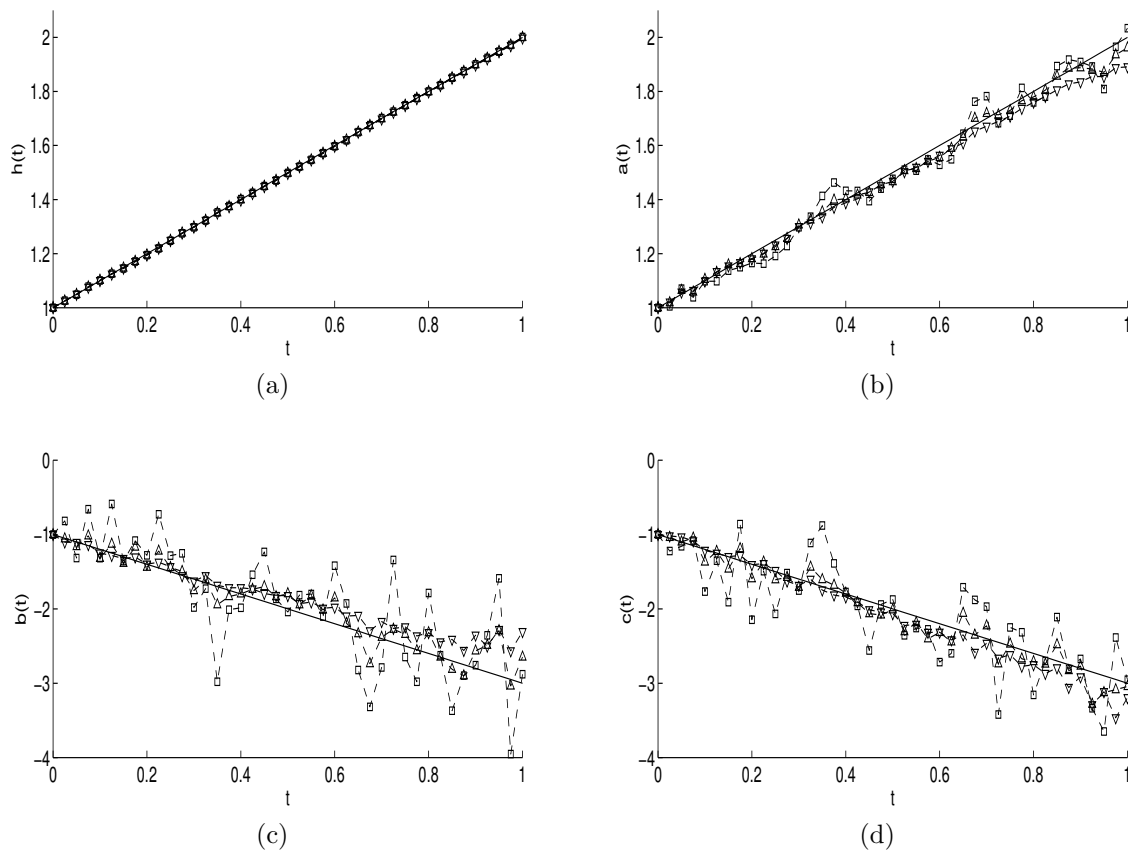


Figure 13: The exact (—) and numerical solutions for: (a) the free boundary $h(t)$, (b) the coefficient $a(t)$, (c) the coefficient $b(t)$, and (d) the coefficient $c(t)$, with regularization parameters $\beta_1 = \beta_2 = 0$, and $\beta_i = 10^{-4}$ ($-\square-$), $\beta_i = 10^{-3}$ ($-\nabla-$), $\beta_i = 10^{-2}$ ($-\triangle-$), $i = 3, 4$, with $p = 0.1\%$ noise for Example 3.

6.2.2 Example 4

Consider now the second inverse problem given by equations (2), (3), (5), (6), (34), (90) and (91) with unknown coefficients $h(t)$, $a(t)$, $b(t)$ and $c(t)$, and solve this problem with the same input data as in Example 3 but replacing $\mu_3(t)$ by $\mu_6(t)$ given by

$$\mu_6(t) = \int_0^{h(t)} x^2 u(x, t) dx = \frac{1}{30}(1+t)^4(31+27t+6t^2), \quad t \in [0, 1].$$

One can remark that the conditions of Theorem 4 are satisfied hence, the unique local solvability of solution holds. The analytical solution is given by equations (101) and (102). All the computational details and numerical representation are the same as those for Example 3 except that noise is now included in the input data $\mu_6(t)$, as well. Figures 14–19, and Tables 4 and 5 represent/ illustrate analogous quantities as Figures 8–13 and Tables 2 and 3 for Example 3 and similar conclusions can be obtained.

It is also possible to compare, at least for the case without noise, the level of information provided to the inverse problem by the Stefan condition (4) in comparison with the second-order heat moment specification (34). Indeed, by comparing Figure 8 and Table 2 with Figure 14 and Table 4, respectively, it can be seen that the rate of convergence is much higher for Example 3 than for Example 4. Moreover, the computational time required to achieve the

converge of the objective functions (99) and (100) is much higher for Example 4 than for Example 3. Finally, by comparing the accuracy of the numerical results presented in Figure 9 and Table 2 of Example 3 with Figure 15 and Table 4 of Example 4, respectively, one can clearly conclude that the Stefan condition (4) provides significantly more information than the second-order heat moment specification (34), especially in predicting the coefficients $b(t)$ and $c(t)$. Similar considerations can also be made for the case of $p = 0.1\%$ noisy data, by comparing Figures 10–13 and Table 3 of Example 3 with Figures 16–19 and Table 5 of Example 4, but this comparison is less reliable because in the latter example we include noise in all the four input data $\tilde{\mu}_3, \mu_4, \mu_5$ and μ_6 , whilst in the former example we include noise only in three input data $\tilde{\mu}_3, \mu_4$ and μ_5 , having the fourth one μ_3 uncontaminated.

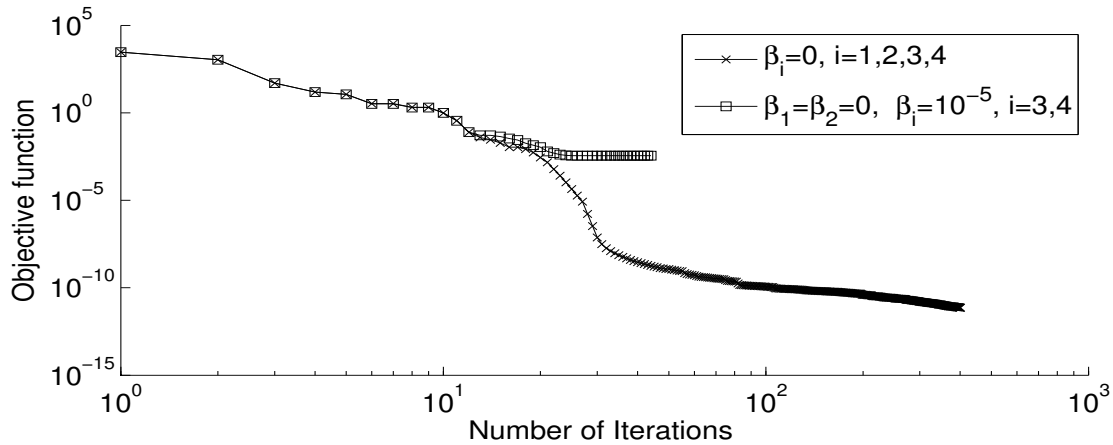


Figure 14: The objective function (100) without noise for Example 4.

Table 4: Number of iterations, number of function evaluations, value of the objective function (100) at final iteration, $rmse$ values (80)-(82) and (104), and the computational time with no noise for Example 4.

$\beta_1 = \beta_2 = 0$	$\beta_3 = \beta_4 = 0$	$\beta_3 = \beta_4 = 10^{-5}$
No. of iterations	401	44
No. of function evaluations	66330	7425
Value of objective function (100) at final iteration	7.2E-12	0.0035
$rmse(h)$	6.1E-4	5.9E-4
$rmse(a)$	0.0058	0.0048
$rmse(b)$	0.1289	0.0847
$rmse(c)$	0.1672	0.0999
Computational time	23 hours	138 min

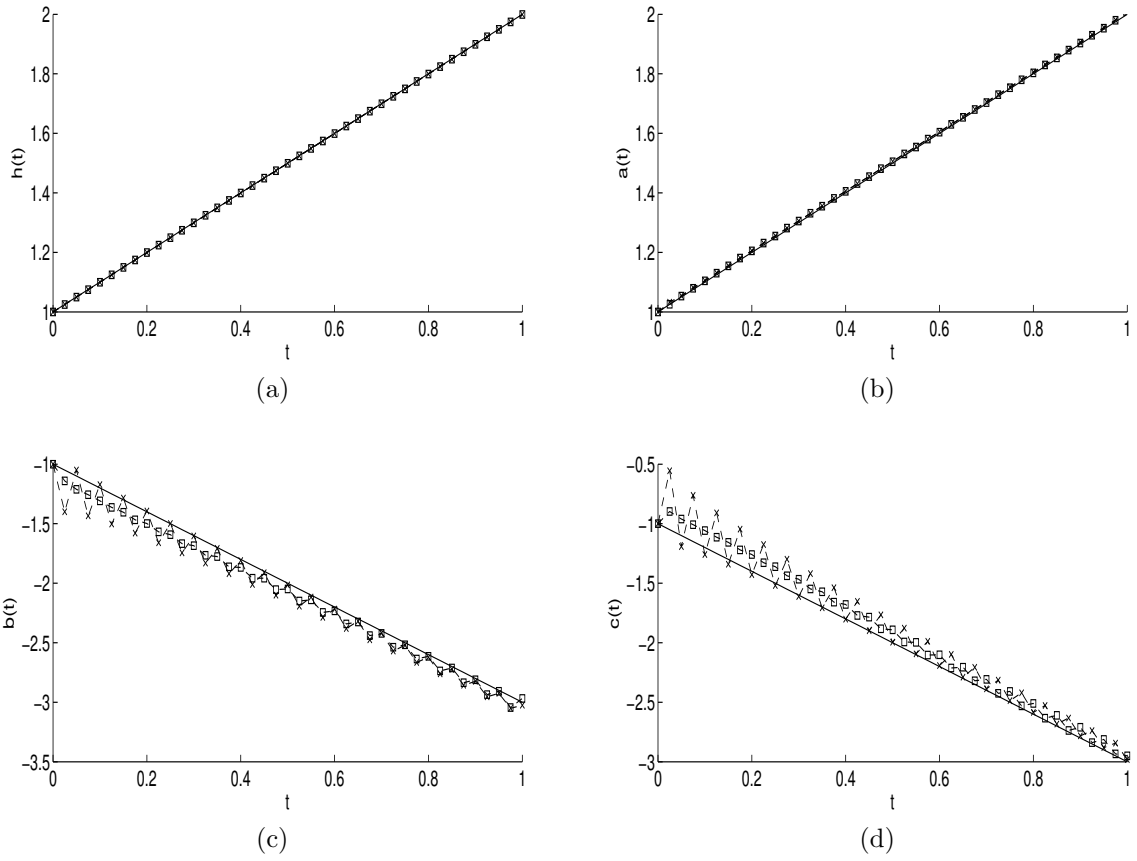


Figure 15: The exact (—) and numerical solutions (—x—) without regularization, and (—□—) with regularization parameters $\beta_1 = \beta_2 = 0$, and $\beta_3 = \beta_4 = 10^{-5}$ for: (a) the free boundary $h(t)$, (b) the coefficient $a(t)$, (c) the coefficient $b(t)$, and (d) the coefficient $c(t)$, without noise for Example 4.

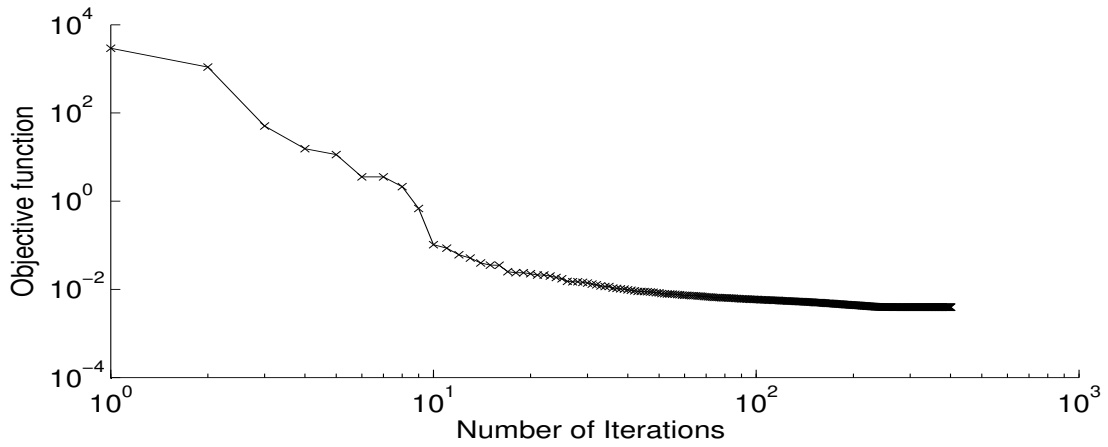


Figure 16: The objective function (100) with $p = 0.1\%$ noise and no regularization for Example 4.

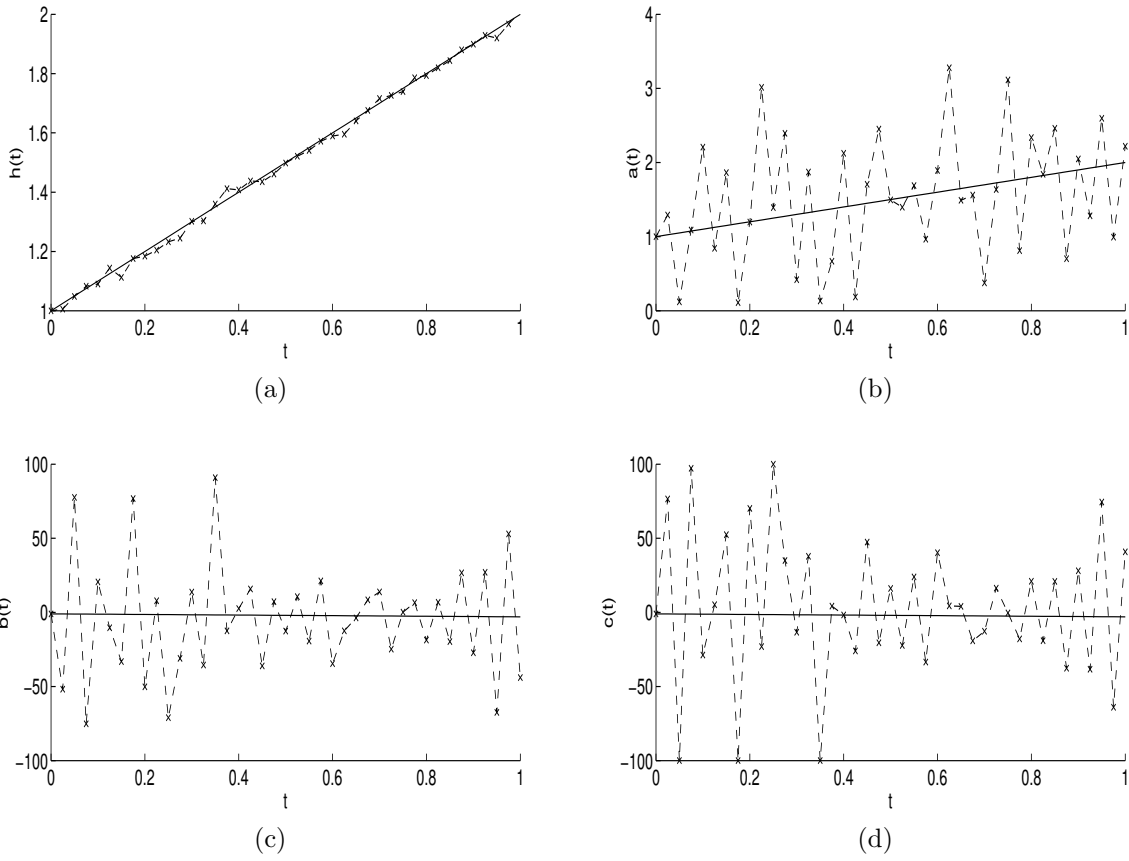


Figure 17: The exact (—) and numerical solutions (—x—) without regularization for: (a) the free boundary $h(t)$, (b) the coefficient $a(t)$, (c) the coefficient $b(t)$, and (d) the coefficient $c(t)$, with $p = 0.1\%$ noise for Example 4.

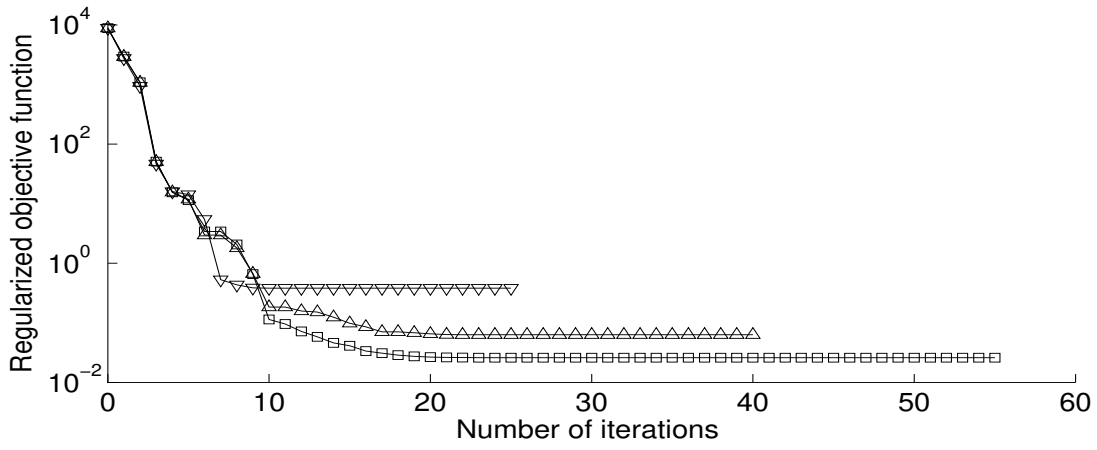


Figure 18: The regularized objective function (100), with regularization parameters $\beta_1 = \beta_2 = 0$, and $\beta_i = 10^{-5}$ (\square -), $\beta_i = 10^{-4}$ (\triangle -), $\beta_i = 10^{-3}$ (∇ -), $i = 3, 4$, with $p = 0.1\%$ noise for Example 4.

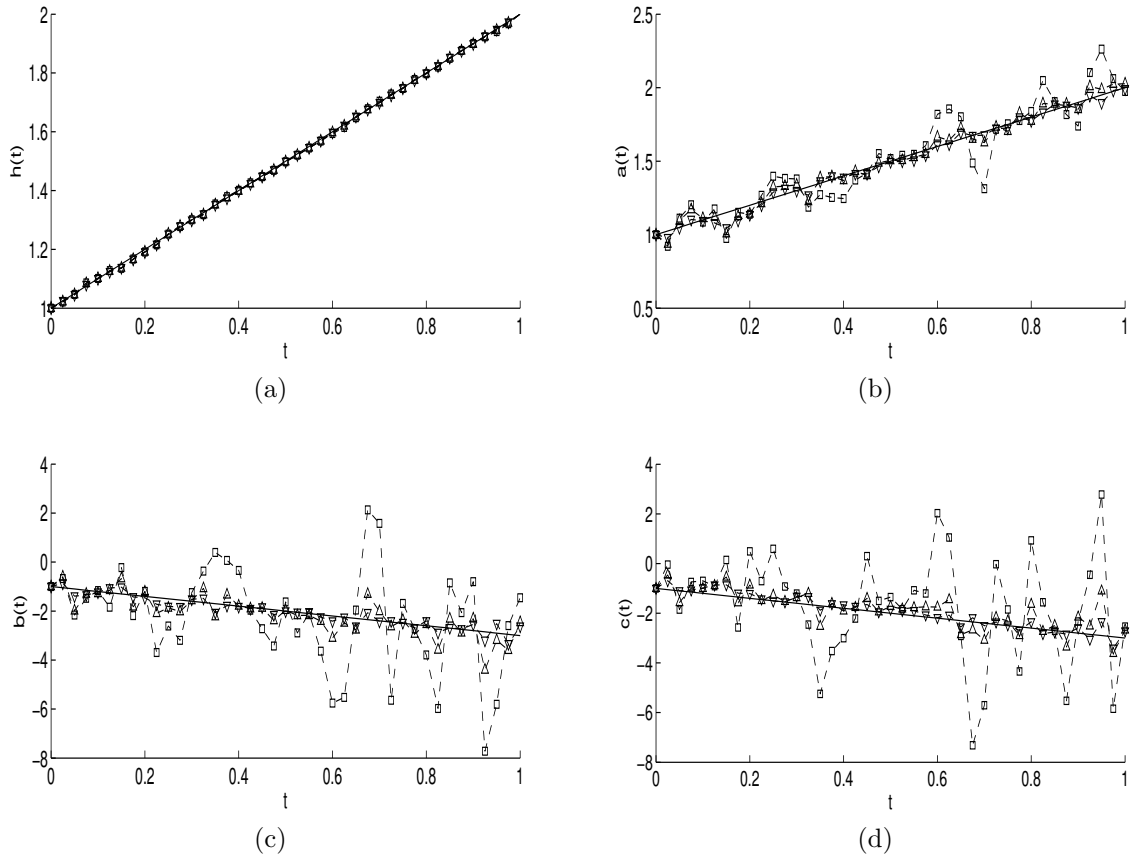


Figure 19: The exact (—) and numerical solutions for: (a) the free boundary $h(t)$, (b) the coefficient $a(t)$, (c) the coefficient $b(t)$, and (d) the coefficient $c(t)$, with regularization parameters $\beta_1 = \beta_2 = 0$, and $\beta_i = 10^{-5}$ ($-\square-$), $\beta_i = 10^{-4}$ ($-\triangle-$), $\beta_i = 10^{-3}$ ($-\nabla-$), $i = 3, 4$, with $p = 0.1\%$ noise for Example 4.

Table 5: Number of iterations, number of function evaluations, value of the objective function (100) at final iteration, $rmse$ values (80)-(82) and (104), and computational time, for $p = 0.1\%$ noise for Example 4.

$\beta_1=0, \beta_2=0$	$\beta_3=\beta_4=0$	$\beta_3=\beta_4=10^{-5}$	$\beta_3=\beta_4=10^{-4}$	$\beta_3=\beta_4=10^{-3}$
No. of iterations	401	55	40	25
No. of function evaluations	66330	9240	6765	5610
Value of objective function (100) at final iteration	0.0039	0.0260	0.0632	0.3820
$rmse(h)$	0.0156	0.0055	0.0044	0.0041
$rmse(a)$	0.8098	0.1338	0.0535	0.0354
$rmse(b)$	37.739	1.9712	0.5126	0.2073
$rmse(c)$	48.118	2.1369	0.5245	0.2218
Computational time	24 hours	150 min	81 min	48 min

7 Conclusions

In this paper, a theoretical and numerical investigation for the recovery of multiple time-dependent coefficients entering the parabolic heat equation with a free boundary has been presented. The moving boundary value problem has been first transformed, by a simple change of variables, to a problem formulated in a fixed domain. Theoretically, new less restrictive conditions for local (in time) unique solvability of solution than the ones in [18] have been proposed. In addition, the Stefan condition can be replaced by a second-order heat moment specification for which the unique solvability has also been proved. The analysis can also be extended to the case when both sides of the finite slab are free, [20, 21].

Numerically, we discretised the governing equation using the FDM and solved the inverse problem as a constrained regularized minimization using the MATLAB optimization routine *lsqnonlin*. Notably, we report that the inclusion of regularization, apart from restoring the stability of the numerical solution, it also reduces the computational time for the minimization using the *lsqnonlin* routine from several hours to several minutes, see Tables 1, 4 and 5. Numerical results presented and discussed for several test examples show that accurate and stable numerical solutions have been achieved. It is also interesting to conclude that, based on the comparison between the Examples 3 and 4, the Stefan condition (4) contains more information than the second-order moment (34).

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