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Determination of the time-dependent convection coefficient in two-dimensional free boundary problems

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Abstract

Purpose. The inverse problem of determining the time-dependent convection coefficient and the free boundary, along with the temperature in the two-dimensional convection-diffusion equation with initial and boundary conditions supplemented by non-local integral observations is, for the first time, numerically solved. From literature we already know that this inverse problem has a unique solution. However, the problem is still ill-posed by being unstable to noise in the input data.
Design/methodology. For the numerical discretisation, we apply the alternating direction explicit finite-difference method along with the Tikhonov regularization to find a stable and accurate numerical solution. The resulting nonlinear minimization problem is solved computationally using the MATLAB routine *lsqnonlin*. Both exact and numerically simulated noisy input data are inverted.
Findings. The numerical results demonstrate that accurate and stable solutions are obtained.
Originality. The inverse problem presented in this paper was already showed to be locally uniquely solvable, but no numerical solution has been realised so far; hence, the main originality of this work is to attempt this task.

Keywords: Inverse problem; Free boundary; Two-dimensional heat equation; Tikhonov regularization; Nonlinear optimization.

1 Introduction

Free boundary problems for parabolic partial differential equations have significant applications in various fields of engineering, physics, chemistry, see [1,3,7–10,12,14] to mention only a few. In particular, the Stefan problem is a moving free boundary problem that concerns the distribution of heat in a phase-change transforming medium. The authors of [3] considered two fairly different free boundary problems of nonlinear diffusion. Chen and Feldman [7] recast the formulation of various shock diffraction/reflection problems as a free boundary problem. Recently, the authors numerically solved several inverse thermal problems concerning the determination time-dependent coefficients along with free boundaries, [8, 9, 12].

There is also an analysis of a one-dimensional inverse problem of reconstructing the timewise heat source with a moving boundary [16]. The authors in [6] estimated free boundary coming from two scenarios, aggregation processes and nonlocal diffusion. Snitko

[19], theoretically, and Huntul [11], numerically, investigated the inverse problem of determining the time-dependent reaction coefficient in a two-dimensional parabolic problem with a free boundary.

The challenge associated with free boundary problems arises from the fact that the solution domain is unknown, and only a few studies focus on the time-dependent free boundary in higher dimensions, e.g. [13, 18, 20, 21]. These papers are theoretical and very important because they present sufficient conditions for the unique solvability of the unknown coefficients. On the other hand, the numerical realization is also very important for practical purposes of application.

This work examines the inverse problem of recovering the time-dependent convection coefficient and free boundaries from nonlocal integral observations as over-specified conditions. Such inverse mathematical modelling is relevant to multiple-phase flow applications in which there exists transient convection that cannot be measured directly or accurately due to inaccessibility or hostile environment. The inverse problem presented in this paper has already been showed to be locally uniquely solvable by Snitko [22], but no numerical solution has been realised so far; hence, the main goal of this work is to attempt this task.

The arrangement of this paper is systematized as follows. Section 2 describes the formulations of the inverse problem. The solution of the direct problem using the alternating direction explicit (ADE) method is presented in Section 3. The ADE direct solver is coupled with the Tikhonov regularization method in Section 4. In Section 5, computational results and discussions are presented. Finally, Section 6 highlights the conclusions.

2 Formulation of the inverse problem

Consider the inverse problem of determining time-dependent convection coefficients $b_1(t)$ and $b_2(t)$, and the free boundaries $l(t) > 0$ and $h(t) > 0$, in the two-dimensional convection-diffusion equation

$$u_t = \nabla^2 u + b_1(t)u_{x_1} + b_2(t)u_{x_2} + f(x_1, x_2, t), \quad (x_1, x_2, t) \in \Omega_T, \tag{1}$$

where $f(x_1, x_2, t)$ is a known heat source, $u = u(x_1, x_2, t)$ is the unknown temperature in the moving domain $\Omega_T := \{(x_1, x_2, t)|\ 0 < x_1 < l(t), 0 < x_2 < h(t), 0 < t < T < \infty\}$, subject to the initial condition

$$u(x_1, x_2, 0) = \varphi(x_1, x_2), \quad (x_1, x_2) \in [0, l_0] \times [0, h_0], \tag{2}$$

where $l_0 \equiv l(0)$ and $h_0 \equiv h(0)$ are given positive numbers, the Dirichlet boundary conditions

$$u(0, x_2, t) = \kappa_1(x_2, t), \quad u(l(t), x_2, t) = \kappa_2(x_2, t), \quad x_2 \in [0, h(t)],\ t \in [0, T], \tag{3}$$

$$u(x_1, 0, t) = \kappa_3(x_1, t), \quad u(x_1, h(t), t) = \kappa_4(x_1, t), \quad x_1 \in [0, l(t)],\ t \in [0, T], \tag{4}$$

and the nonlocal integral observations

$$l'(t) + \int_0^{h(t)} u_{x_1}(l(t), x_2, t)dx_2 = \kappa_5(t), \quad t \in [0, T], \tag{5}$$

$$h'(t) + \int_0^{l(t)} u_{x_2}(x_1, h(t), t)dx_1 = \kappa_6(t), \quad t \in [0, T], \tag{6}$$

$$\int_0^{l(t)} \int_0^{h(t)} u(x_1, x_2, t) dx_2 dx_1 = \kappa_7(t), \quad t \in [0, T], \tag{7}$$

$$\int_0^{l(t)} \int_0^{h(t)} x_2 u(x_1, x_2, t) dx_2 dx_1 = \kappa_8(t), \quad t \in [0, T], \tag{8}$$

where φ and κ_i for $i = \overline{1, 8}$ are given functions satisfying compatibility conditions. The functions $\kappa_5(t)$ and $\kappa_6(t)$ in (5) and (6) represent Stefan integral boundary conditions. The function $\kappa_7(t)$ in (7) corresponds to the specification of mass/energy, [4,5], whilst the function $\kappa_8(t)$ in (8) represents the first-order moment specification, [17]. In the above inverse formulation we are concerned with the stable invertibility of the map $(b_1, b_2, l, h) \mapsto (k_5, k_6, k_7, k_8)$ in suitable spaces of admissible functions. Problems of the above type (1)-(8) arise in the mathematical modelling of free boundaries in melting or ablation, and in the oil and gas production during drilling and operation of wells, [23].

Using that for arbitrary continuously differentiable functions $q(\zeta, t)$ and $\chi(t)$ we have

$$\frac{d}{dt}\left(\int_0^{\chi(t)} q(\zeta, t) d\zeta \right) = \int_0^{\chi(t)} q_t(\zeta, t) d\zeta + \chi'(t) q(\chi(t), t),$$

we get from (7) by differentiation that:

$$\kappa_7'(t) = \int_0^{l(t)} \int_0^{h(t)} u_t(x_1, x_2, t) dx_2 dx_1 + l'(t) \int_0^{h(t)} u(l(t), x_2, t) dx_2$$
$$+ h'(t) \int_0^{l(t)} u(x_1, h(t), t) dx_1 = \int_0^{l(t)} \int_0^{h(t)} u_t(x_1, x_2, t) dx_2 dx_1 + l'(t) \int_0^{h(t)} \kappa_2(x_2, t) dx_2$$
$$+ h'(t) \int_0^{l(t)} \kappa_4(x_1, t) dx_1 = l'(t) \int_0^{h(t)} \kappa_2(x_2, t) dx_2 + h'(t) \int_0^{l(t)} \kappa_4(x_1, t) dx_1$$
$$+ \int_0^{l(t)} \int_0^{h(t)} \left[\nabla^2 u(x_1, x_2, t) + f(x_1, x_2, t) \right] dx_1 dx_2$$
$$+ b_1(t) \int_0^{h(t)} \Big(\kappa_2(x_2, t) - \kappa_1(x_2, t) \Big) dx_2 + b_2(t) \int_0^{l(t)} \Big(\kappa_4(x_1, t) - \kappa_3(x_1, t) \Big) dx_1. \tag{9}$$

Similarly, differentiating (8) we obtain

$$\kappa_8'(t) = l'(t) \int_0^{h(t)} x_2 \kappa_2(x_2, t) dx_2 + h'(t) h(t) \int_0^{l(t)} \kappa_4(x_1, t) dx_1$$
$$+ \int_0^{l(t)} \int_0^{h(t)} x_2 \left[\nabla^2 u(x_1, x_2, t) + f(x_1, x_2, t) \right] dx_1 dx_2$$
$$+ b_1(t) \int_0^{h(t)} x_2 \Big(\kappa_2(x_2, t) - \kappa_1(x_2, t) \Big) dx_2 + b_2(t) \left[h(t) \int_0^{l(t)} \kappa_4(x_1, t) dx_1 - \kappa_7(t) \right]. \tag{10}$$

Applying equations (5), (6), (9) and (10) at $t = 0$ and using the compatibility between the initial data (2) and the Dirichlet boundary conditions (3) and (4) we obtain:

$$l'(0) = \kappa_5(0) - \int_0^{h_0} \varphi_{x_1}(l_0, x_2) dx_2, \quad h'(0) = \kappa_6(0) - \int_0^{l_0} \varphi_{x_2}(x_1, h_0) dx_1, \tag{11}$$

$$\kappa_7'(0) = l'(0)\int_0^{h_0} \kappa_2(x_2,0)dx_2 + h'(0)\int_0^{l_0} \kappa_4(x_1,0)dx_1 + \int_0^{l_0}\int_0^{h_0} \left[\nabla^2\varphi(x_1,x_2) + f(x_1,x_2,0)\right] dx_1dx_2$$

$$+b_1(0)\int_0^{h_0} \left[\kappa_2(x_2,0) - \kappa_1(x_2,0)\right] dx_2 + b_2(0)\int_0^{l_0} \left[\kappa_4(x_1,0) - \kappa_3(x_1,0)\right] dx_1, \tag{12}$$

$$\kappa_8'(0) = l'(0)\int_0^{h_0} x_2\kappa_2(x_2,0)dx_2 + h'(0)h_0\int_0^{l_0} \kappa_4(x_1,0)dx_1 + \int_0^{l_0}\int_0^{h_0} x_2\left[\nabla^2\varphi(x_1,x_2) + f(x_1,x_2,0)\right] dx_1dx_2$$

$$+b_1(0)\int_0^{h_0} x_2\left[\kappa_2(x_2,0) - \kappa_1(x_2,0)\right] dx_2 + b_2(0)\left[h_0\int_0^{h_0} \kappa_4(x_1,0)dx_1 - \kappa_7(0)\right]. \tag{13}$$

Then, the values of $l'(0)$, $h'(0)$, $b_1(0)$ and $b_2(0)$ are available from the system of equations (11)–(13).

Introducing the new variables $y_1 = \frac{x_1}{l(t)}$ and $y_2 = \frac{x_2}{h(t)}$, see [22], we recast the problem given by equations (1)–(8) into the problem given below for the unknowns $l(t)$, $h(t)$, $b_1(t)$, $b_2(t)$ and $v(y_1,y_2,t) := u(y_1l(t), y_2h(t), t)$, namely,

$$v_t = \frac{1}{l^2(t)}v_{y_1y_1} + \frac{1}{h^2(t)}v_{y_2y_2} + \left(\frac{b_1(t) + y_1l'(t)}{l(t)}\right)v_{y_1} + \left(\frac{b_2(t) + y_2h'(t)}{h(t)}\right)v_{y_2} + f(y_1l(t), y_2h(t), t),\ (y_1,y_2,t) \in Q_T, \tag{14}$$

where $Q_T := \{(y_1,y_2,t)|\ 0 < y_1 < 1, 0 < y_2 < 1, 0 < t < T\}$ is fixed domain and

$$v(y_1,y_2,0) = \varphi(y_1l_0, y_2h_0),\quad (y_1,y_2) \in [0,1]\times[0,1], \tag{15}$$

$$v(0,y_2,t) = \kappa_1(y_2h(t),t),\quad v(1,y_2,t) = \kappa_2(y_2h(t),t),\quad y_2 \in [0,1],\ t \in [0,T], \tag{16}$$

$$v(y_1,0,t) = \kappa_3(y_1l(t),t),\quad v(y_1,1,t) = \kappa_4(y_1l(t),t),\quad y_1 \in [0,1],\ t \in [0,T], \tag{17}$$

$$l'(t) + \frac{h(t)}{l(t)}\int_0^1 v_{y_1}(1,y_2,t)dy_2 = \kappa_5(t),\quad t \in [0,T], \tag{18}$$

$$h'(t) + \frac{l(t)}{h(t)}\int_0^1 v_{y_2}(y_1,1,t)dy_1 = \kappa_6(t),\quad t \in [0,T], \tag{19}$$

$$l(t)h(t)\int_0^1\int_0^1 v(y_1,y_2,t)dy_2dy_1 = \kappa_7(t),\quad t \in [0,T], \tag{20}$$

$$l(t)h^2(t)\int_0^1\int_0^1 y_2v(y_1,y_2,t)dy_2dy_1 = \kappa_8(t),\quad t \in [0,T]. \tag{21}$$

The local existence and uniqueness of the solution of problem (14)–(21) were established in [22] and read as follows.

Theorem 1. *Suppose that the following conditions are satisfied:*
(A1) $\varphi \in C^2([0,\infty)^2)$, $\kappa_i \in C^{2,1}([0,\infty)\times[0,T])$ *for* $i = \overline{1,4}$, $\kappa_i \in C[0,T]$ *for* $i = 5,6$, $\kappa_i \in C^1[0,T]$ *for* $i = 7,8$, $0 \le f \in C^{1,0}([0,\infty)^2\times[0,T])$;
(A2) $0 < \varphi_0 \le \varphi(x_1,x_2) \le \varphi_1 < \infty$ *for* $(x_1,x_2) \in [0,\infty)^2$, $\varphi_{x_1}(x_1,x_2) > 0$, $\varphi_{x_2}(x_1,x_2) >$

0 for $(x_1, x_2) \in [0, l_0] \times [0, h_0], \varphi_{x_1}(x_1, x_2) - \varphi_{x_1}(x_1, h_0 - x_2) > 0$, $\varphi_{x_2}(x_1, h_0 - x_2) - \varphi_{x_2}(x_1, x_2) > 0$ for $(x_1, x_2) \in [0, l_0] \times [0, h_0/2)$, $\kappa_i(t) > 0$ for $t \in [0, T]$ and $i = 7, 8$;
(A3) compatibility conditions of the zeroth and first order.
Then, it is possible to indicate a time $T_0 \in (0, T]$, determined by the input data, such that there exists a solution $(l(t), h(t), b_1(t), b_2(t), v(y_1, y_2, t)) \in (C^1[0, T_0])^2 \times (C[0, T_0])^2 \times C^{2,1}(\overline{Q}_{T_0})$ with $l(t) > 0$, $h(t) > 0$ for $t \in [0, T_0]$, to problem (14)–(21).

Theorem 2. *Suppose that in addition to (A2) the following condition is satisfied:*
(A4) $f \in C^{1,0}([0, \infty)^2 \times [0, T])$, $\varphi \in C^2([0, \infty)^2)$, $\kappa_i \in C^{3,1}([0, \infty) \times [0, T])$ for $i = \overline{1, 4}$.
Then, it is possible to indicate a time $T_1 \in (0, T]$, determined by the input data, such that problem (14)–(21) has at most one solution $(l(t), h(t), b_1(t), b_2(t), v(y_1, y_2, t)) \in (C^1[0, T_1])^2 \times (C[0, T_1])^2 \times C^{2,1}(\overline{Q}_{T_1})$ with $l(t) > 0$, $h(t) > 0$ for $t \in [0, T_1]$.

Although Theorems 1 and 2 guarantee the local existence and uniqueness of the solution, the inverse problem is still ill-posed because small rando errors into the input data cause large errors in the output solution, As it will be described in Section 4, special methods of optimization based on the nonlinear Tikhononv's regularization method need to be employed in order to restore stability of the solution. But before we do that, the next section describes the forward solver for the well-posed linear direct problem which needs to be employed iteratively to obtain the solution of the ill-posed non-linear inverse problem.

3 Forward solver for the time-dependent convection-diffusion equation

Now, consider the direct (forward) problem (14)–(17). When $l(t)$, $h(t)$, $b_1(t)$, $b_2(t)$, $f(x_1, x_2, t)$, $\kappa_i(t)$ for $i = \overline{1, 4}$, and $\varphi(x_1, x_2)$ are given in the direct problem $v(y_1, y_2, t)$ is to be found along with the quantities of interest $\kappa_i(t)$ for $i = \overline{5, 8}$. Denote $v(y_1, y_2, t_n) = v^n_{i,j}$, $l(t_n) = l_n$, $h(t_n) = h_n$, $b_1(t_n) = b_{1_n}$, $b_2(t_n) = b_{2_n}$ and $f(y_1 l(t_n), y_2 h(t_n), t_n) = f^n_{i,j}$, where $y_{1i} = i\Delta y_1$, $y_{2j} = j\Delta y_2$, $t_n = n\Delta t$, $\Delta y_1 = 1/M_1$, $\Delta y_2 = 1/M_2$, $\Delta t = T/N$ for $i = \overline{0, M_1}$, $j = \overline{0, M_2}$, $n = \overline{0, N}$.

The ADE method, [2, 10], which is unconditionally stable, is described for solving numerically the direct problem (14)–(17). Let $\tilde{v}^n_{i,j}$ and $\tilde{u}^n_{i,j}$ satisfy

$$\begin{aligned}\tilde{v}^{n+1}_{i,j} &= A_n \tilde{v}^n_{i,j} + B_n(\tilde{v}^n_{i+1,j} + \tilde{v}^{n+1}_{i-1,j}) + C_n(\tilde{v}^n_{i,j+1} + \tilde{v}^{n+1}_{i,j-1}) + D_n(\tilde{v}^n_{i+1,j} - \tilde{v}^{n+1}_{i-1,j}) \\ &\quad + E_n(\tilde{v}^n_{i,j+1} - \tilde{v}^{n+1}_{i,j-1}) + G^*_{i,j}, \ i = \overline{1, M_1 - 1}, \ j = \overline{1, M_2 - 1}, \ n = \overline{0, N - 1}, \end{aligned} \tag{22}$$

$$\begin{aligned}\tilde{u}^{n+1}_{i,j} &= A_n \tilde{u}^n_{i,j} + B_n(\tilde{u}^{n+1}_{i+1,j} + \tilde{u}^n_{i-1,j}) + C_n(\tilde{u}^{n+1}_{i,j+1} + \tilde{u}^n_{i,j-1}) + D_n(\tilde{u}^{n+1}_{i+1,j} - \tilde{u}^n_{i-1,j}) \\ &\quad + E_n(\tilde{u}^{n+1}_{i,j+1} - \tilde{u}^n_{i,j-1}) + G^*_{i,j}, \ i = \overline{M_1 - 1, 1}, \ j = \overline{M_2 - 1, 1}, \ n = \overline{0, N - 1}, \end{aligned} \tag{23}$$

where

$$\begin{aligned} A_n &= \frac{1 - \lambda_n}{1 + \lambda_n}, \quad B_n = \frac{\Delta t}{l_n^2 (\Delta y_1)^2 (1 + \lambda_n)}, \quad C_n = \frac{\Delta t}{h_n^2 (\Delta y_2)^2 (1 + \lambda_n)}, \\ D_n &= \frac{\Delta t}{2\Delta y_1} \left(\frac{b_{1_n} + y_{1i} l'_n}{l_n (1 + \lambda_n)} \right), \quad E_n = \frac{\Delta t}{2\Delta y_2} \left(\frac{b_{2_n} + y_{2j} h'_n}{h_n (1 + \lambda_n)} \right), \\ G^*_{i,j} &= \frac{\Delta t}{2(1 + \lambda^n_{i,j})} \left(f^{n+1}_{i,j} + f^n_{i,j} \right), \quad \lambda_n = \frac{\Delta t}{l_n^2 (\Delta y_1)^2} + \frac{\Delta t}{h_n^2 (\Delta y_2)^2}. \end{aligned} \tag{24}$$

Furthermore, let the $\tilde{v}^n_{i,j}$ and $\tilde{u}^n_{i,j}$ also satisfy the initial and boundary conditions (15)–(17), namely,

$$\tilde{v}^0_{i,j} = \tilde{u}^0_{i,j} = \varphi_{i,j}, \quad i = \overline{0, M_1}, \quad j = \overline{0, M_2}, \tag{25}$$

$$\tilde{v}^n_{0,j} = \tilde{u}^n_{0,j} = \kappa_1(y_{2j}h_n, t_n), \quad \tilde{v}^n_{M_1,j} = \tilde{u}^n_{M_1,j} = \kappa_2(y_{2j}h_n, t_n), \quad j = \overline{0, M_2}, \quad n = \overline{1, N}, \tag{26}$$

$$\tilde{v}^n_{i,0} = \tilde{u}^n_{i,0} = \kappa_3(y_{1i}l_n, t_n), \quad \tilde{v}^n_{i,M_2} = \tilde{u}^n_{i,M_2} = \kappa_4(y_{1i}l_n, t_n), \quad i = \overline{0, M_1}, \quad n = \overline{1, N}. \tag{27}$$

Once $\tilde{v}^{n+1}_{i,j}$ and $\tilde{u}^{n+1}_{i,j}$ have been obtained, the solution of the direct problem (14)–(17) is computed by

$$v^{n+1}_{i,j} = \frac{\tilde{v}^{n+1}_{i,j} + \tilde{u}^{n+1}_{i,j}}{2}. \tag{28}$$

The trapezoidal rule is used to approximate all the integrals in (18)–(21), as follows:

$$l'(t_n) + \frac{h(t_n)}{l(t_n)} \int_0^1 v_{y_1}(1, y_2, t_n) dy_2 = l'_n + \frac{h_n}{l_n} \left[\frac{1}{2M_2} \Big(v_{y_1}(1, 0, t_n) + v_{y_1}(1, 1, t_n) + 2 \sum_{j=1}^{M_2-1} v_{y_1}(1, y_{2j}, t_n) \Big) \right], \quad n = \overline{1, N}, \tag{29}$$

where

$$v_{y_1}(1, 0, t_n) = \frac{4v(y_{1_{M_1-1}}, y_2, t_n) - v(y_{1_{M_1-2}}, y_2, t_n) - 3v(y_{1_{M_1}}, y_2, t_n)}{-2(\Delta y_1)}, \quad n = \overline{1, N},$$

$$v_{y_1}(1, 1, t_n) = \frac{4v(y_{1_{M_1-1}}, y_{2_{M_2-1}}, t_n) - v(y_{1_{M_1-2}}, y_{2_{M_2-2}}, t_n) - 3v(y_{1_{M_1}}, y_{2_{M_2}}, t_n)}{-2(\Delta y_1)}, \quad n = \overline{1, N},$$

$$v_{y_1}(1, y_{2j}, t_n) = \frac{4v(y_{1_{M_1-1}}, y_{2j}, t_n) - v(y_{1_{M_1-2}}, y_{2j}, t_n) - 3v(y_{1_{M_1}}, y_{2j}, t_n)}{-2(\Delta y_1)}, \quad j = \overline{1, M_2 - 1} \quad n = \overline{1, N},$$

$$h'(t_n) + \frac{l(t_n)}{h(t_n)} \int_0^1 v_{y_2}(y_1, 1, t_n) dy_1 = h'_n + \frac{l_n}{h_n} \left[\frac{1}{2M_1} \Big(v_{y_2}(0, 1, t_n) + v_{y_2}(1, 1, t_n) + 2 \sum_{i=1}^{M_1-1} v_{y_2}(y_{1i}, 1, t_n) \Big) \right], \quad n = \overline{1, N}, \tag{30}$$

where

$$v_{y_2}(0, 1, t_n) = \frac{4v(y_1, y_{2_{M_2-1}}, t_n) - v(y_1, y_{2_{M_2-2}}, t_n) - 3v(y_1, y_{2_{M_2}}, t_n)}{-2(\Delta y_2)}, \quad n = \overline{1, N},$$

$$v_{y_2}(1,1,t_n) = \frac{4v(y_{1_{M_1-1}}, y_{2_{M_2-1}}, t_n) - v(y_{1_{M_1-2}}, y_{2_{M_2-2}}, t_n) - 3v(y_{1_{M_1}}, y_{2_{M_2}}, t_n)}{-2(\Delta y_2)},$$
$$n = \overline{1, N},$$

$$v_{y_2}(y_{1i},1,t_n) = \frac{4v(y_{1i}, y_{2_{M_2-1}}, t_n) - v(y_{1i}, y_{2_{M_2-2}}, t_n) - 3v(y_{1i}, y_{2_{M_2}}, t_n)}{-2(\Delta y_2)},$$
$$i = \overline{1, M_1-1}, \quad n = \overline{1, N},$$

$$l(t_n)h(t_n)\int_0^1\int_0^1 v(y_1,y_2,t_n)dy_2dy_1 = \frac{l_nh_n}{4M_1M_2}\Bigg[v(0,0,t_n)+v(1,0,t_n)$$
$$+v(0,1,t_n)+v(1,1,t_n)+2\sum_{i=1}^{M_1-1}v(y_{1i},0,t_n)+2\sum_{i=1}^{M_1-1}v(y_{1i},1,t_n)$$
$$+2\sum_{j=1}^{M_2-1}v(0,y_{2j},t_n)+2\sum_{j=1}^{M_2-1}v(1,y_{2j},t_n)+4\sum_{j=1}^{M_2-1}\sum_{i=1}^{M_1-1}v(y_{1i},y_{2j},t_n)\Bigg], \quad n=\overline{1,N},$$

$$l(t_n)h^2(t_n)\int_0^1\int_0^1 y_2v(y_1,y_2,t_n)dy_2dy_1 = \frac{l_nh_n^2}{4M_1M_2}\Bigg[y_2(0)v(0,0,t_n)+y_2(0)v(1,0,t_n)$$
$$+y_2(1)v(0,1,t_n)+y_2(1)v(1,1,t_n)+2\sum_{i=1}^{M_1-1}y_2(0)v(y_{1i},0,t_n)+2\sum_{i=1}^{M_1-1}y_2(1)v(y_{1i},1,t_n)$$
$$+2\sum_{j=1}^{M_2-1}y_{2j}v(0,y_{2j},t_n)+2\sum_{j=1}^{M_2-1}y_{2j}v(1,y_{2j},t_n)+4\sum_{j=1}^{M_2-1}\sum_{i=1}^{M_1-1}y_{2j}v(y_{1i},y_{2j},t_n)\Bigg],$$
$$n=\overline{1,N}.$$

4 Solution of the inverse problem

We want to find stable and accurate reconstructions of $l(t)$, $h(t)$, $b_1(t)$, $b_2(t)$ and $v(y_1, y_2, t)$ satisfying the nonlinear and ill-posed inverse problem (14)–(21). This is achieved by minimizing the regularized objective function

$$\begin{aligned} F(l,h,b_1,b_2) = &\left\| l'(t) + \frac{h(t)}{l(t)}\int_0^1 v_{y_1}(1,y_2,t)dy_2 - \kappa_5(t)\right\|^2 \\ &+ \left\| h'(t) + \frac{l(t)}{h(t)}\int_0^1 v_{y_2}(y_1,1,t)dy_1 - \kappa_6(t)\right\|^2 \\ &+ \left\| l(t)h(t)\int_0^1\int_0^1 v(y_1,y_2,t)dy_2dy_1 - \kappa_7(t)\right\|^2 \\ &+ \left\| l(t)h^2(t)\int_0^1\int_0^1 y_2v(y_1,y_2,t)dy_2dy_1 - \kappa_8(t)\right\|^2 \\ &+ \lambda_1||l(t)||^2+\lambda_2||h(t)||^2+\lambda_3||b_1(t)||^2+\lambda_4||b_2(t)||^2, \end{aligned} \tag{31}$$

where v solves (14)–(17) for given (l, h, b_1, b_2), and $\lambda_i \geq 0$ for $i = \overline{1,4}$ are regularization parameters to be prescribed, and the norm is the $L^2(0,T)$-norm. As it will turn out from the insight gained from the numerical investigation in Section 4, the free boundary $(l(t), h(t))$ is obtained to be stable with respect to noise in the input data (18)–(21); hence we can safely take $\lambda_1 = \lambda_2 = 0$ in (31). In the expressions (29), (30) and (31), we approximate the derivatives of $l(t)$ and $h(t)$ as

$$l'_n := l'(t_n) \approx \frac{l(t_n) - l(t_{n-1})}{\Delta t} = \frac{l_n - l_{n-1}}{\Delta t}, \quad n = \overline{1,N}, \tag{32}$$

$$h'_n := h'(t_n) \approx \frac{h(t_n) - h(t_{n-1})}{\Delta t} = \frac{h_n - h_{n-1}}{\Delta t}, \quad n = \overline{1,N}. \tag{33}$$

In discrete form, equation (31) becomes

$$\begin{aligned} F(\mathbf{l}, \mathbf{h}, \mathbf{b_1}, \mathbf{b_2}) = & \sum_{n=1}^{N} \left[\frac{l_n - l_{n-1}}{\Delta t} + \frac{h_n}{l_n} \int_0^1 v_{y_1}(1, y_2, t_n) dy_2 - \kappa_5(t_n) \right]^2 \\ & + \sum_{n=1}^{N} \left[\frac{h_n - h_{n-1}}{\Delta t} + \frac{l_n}{h_n} \int_0^1 v_{y_2}(y_1, 1, t_n) dy_1 - \kappa_6(t_n) \right]^2 \\ & + \sum_{n=1}^{N} \left[l_n h_n \int_0^1 \int_0^1 v(y_1, y_2, t_n) dy_2 dy_1 - \kappa_7(t_n) \right]^2 \\ & + \sum_{n=1}^{N} \left[l_n h_n^2 \int_0^1 \int_0^1 y_2 v(y_1, y_2, t_n) dy_2 dy_1 - \kappa_8(t_n) \right]^2 \\ & + \lambda_1 \sum_{n=1}^{N} l_n^2 + \lambda_2 \sum_{n=1}^{N} h_n^2 + \lambda_3 \sum_{n=1}^{N} b_{1_n}^2 + \lambda_4 \sum_{n=1}^{N} b_{2_n}^2. \end{aligned} \tag{34}$$

The minimization of the objective function (34) is carried out using the MATLAB subroutine *lsqnonlin*. Alternative numerical methods that can be used to efficiently solve optimization problems include the well-known adjoint technique, see e.g. [24] which deals with similar inverse problems for time-dependent partial differential equations.

The inverse problem (14)–(21) is solved with exact as well as noisy data (18)–(21). The noisy data are numerically simulated as

$$\kappa_i^{noise}(t_n) = \kappa_i(t_n) + \epsilon_n, \quad i = \overline{5,8}, \quad n = \overline{1,N}, \tag{35}$$

where ϵ_n are random variables with zero mean and standard deviation

$$\sigma_i = p \times \max_{t \in [0,T]} |\kappa_i(t)|, \quad i = \overline{5,8}, \tag{36}$$

where p denotes the percentage of noise. We utilize the MATLAB function *normrnd* to generate $\underline{\epsilon} = (\epsilon_n)_{n=\overline{1,N}}$ as $\underline{\epsilon} = normrnd(0, \sigma, N)$. In the case of noisy data (35), we replace in (34) $\kappa_i(t_n)$ by $\kappa_i^{noise}(t_n)$ for $i = \overline{5,8}$.

5 Numerical results and discussion

The following root mean square (RMS) errors are defined as

$$\mathrm{RMS}(l) = \left[\frac{T}{N}\sum_{n=1}^{N}\left(l^{numerical}(t_n) - l^{exact}(t_n)\right)^2\right]^{1/2}, \tag{37}$$

$$\mathrm{RMS}(h) = \left[\frac{T}{N}\sum_{n=1}^{N}\left(h^{numerical}(t_n) - h^{exact}(t_n)\right)^2\right]^{1/2}, \tag{38}$$

and similar expressions exist for $b_1(t)$ and $b_2(t)$. We take $T = 1$, for simplicity. Furthermore, we take the lower and upper bounds for $l(t) > 0$ and $h(t) > 0$ to be 10^{-6} and 10^3, respectively, and the lower and upper bounds for the quantities $b_1(t)$ and $b_2(t)$, to be -10^3 and 10^3, respectively. These bounds allow for a wide search range of the unknowns.

Let us investigate the inverse problem (1)–(8) with the input data:

$$\varphi(x_1, x_2) = \frac{3}{2} + \tanh(x_1) - \frac{\cos\left(\frac{\pi x_2}{2} + \frac{\pi}{8}\right)}{1 + x_1}, \quad \kappa_1(x_2, t) = t + \frac{3}{2} - \cos\left(\frac{\pi x_2}{2} + \frac{\pi}{8}\right),$$

$$\kappa_2(x_2, t) = t + \frac{3}{2} + \tanh(1 + t) - \frac{\cos\left(\frac{\pi x_2}{2} + \frac{\pi}{8}\right)}{2 + t}, \quad \kappa_3(x_1, t) = t + \frac{3}{2} + \tanh(x_1)$$

$$-\frac{\cos\left(\frac{\pi}{8}\right)}{1 + x_1}, \quad \kappa_4(x_1, t) = t + \frac{3}{2} + \tanh(x_1) - \frac{\cos\left(\frac{\pi(1+t)}{2} + \frac{\pi}{8}\right)}{1 + x_1}, \quad f(x_1, x_2, t) = 1$$

$$+\frac{2\tanh(x_1) + 2 - \cos(2\pi t)}{\cosh^2(x_1)} + \frac{\cos\left(\frac{\pi x_2}{2} + \frac{\pi}{8}\right)}{1 + x_1}\left[\frac{2}{(1 + x_1)^2} - \frac{\pi^2}{4} + \frac{2 - \cos(2\pi t)}{1 + x_1}\right]$$

$$+\frac{\pi}{2}\sin\left(\frac{\pi x_2}{2} + \frac{\pi}{8}\right)\left(\frac{2 - \cos(2\pi t)}{1 + x_1}\right),$$

$$\kappa_5(t) = 1 + \frac{1 + t}{\cosh^2(1 + t)} + \frac{2}{\pi(2 + t)^2}\left[\cos\left(\frac{\pi t}{2} + \frac{\pi}{8}\right) - \sin\left(\frac{\pi}{8}\right)\right],$$

$$\kappa_6(t) = 1 + \frac{\pi}{2}\cos\left(\frac{\pi t}{2} + \frac{\pi}{8}\right)\ln(2 + t),$$

$$\kappa_7(t) = \frac{2}{\pi}\left[\sin\left(\frac{\pi}{8}\right) - \cos\left(\frac{\pi t}{2} + \frac{\pi}{8}\right)\right]\ln(2 + t) + (1 + t)\ln(\cosh(1 + t)) + \left(\frac{3}{2} + t\right)(1 + t)^2,$$

$$\kappa_8(t) = \frac{2}{\pi^2}\left[2\cos\left(\frac{\pi}{8}\right) - \pi(1 + t)\cos\left(\frac{\pi t}{2} + \frac{\pi}{8}\right) + 2\sin\left(\frac{\pi t}{2} + \frac{\pi}{8}\right)\right]\ln(2 + t)$$

$$+\frac{(1 + t)^2\ln(\cosh(1 + t))}{2} + \frac{(2t^3 + 7t^2 + 8t + 3)(1 + t)}{4}.$$

We observe that the conditions (A1)-(A4) of Theorems 1 and 2 are fulfilled and thus, the existence and uniqueness of the solution are ensured. It can be easily verified that the exact solution of (1)–(8) is

$$u(x_1, x_2, t) = t + \frac{3}{2} + \tanh(x_1) - \frac{\cos\left(\frac{\pi x_2}{2} + \frac{\pi}{8}\right)}{1 + x_1}, \quad (x_1, x_2, t) \in \Omega_T, \tag{39}$$

and

$$l(t) = 1 + t,\ h(t) = 1 + t,\ b_1(t) = -2 + \cos(2\pi t),\ b_2(t) = -2 + \cos(2\pi t),\ t \in [0, 1]. \quad (40)$$

Also,

$$v(y_1, y_2, t) = u(y_1 l(t), y_2 h(t), t) = t + \frac{3}{2} + \tanh(y_1(1+t)) - \frac{\cos\left(\frac{\pi y_2(1+t)}{2} + \frac{\pi}{8}\right)}{1 + y_1(1+t)},$$
$$(y_1, y_2, t) \in Q_T. \quad (41)$$

First, we investigate the accuracy of the direct problem (1)–(4) with the input data (39) when $l(t)$, $h(t)$, $b_1(t)$, $b_2(t)$ are known and given by (40). Table 1 reveals that the exact and numerical solutions for the quantities (18)–(21), obtained with the the finite-difference grids $M_1 = M_2 = 10$ and $N \in \{20, 40, 80\}$ are in good agreement the accuracy increasing, as the mesh size decreases.

Table 1: The numerical and analytical (exact) solutions for $\kappa_i(t)$ for $i = \overline{5, 8}$, obtained with $M_1 = M_2 = 10$ and various $N \in \{20, 40, 80\}$.

t	0.1	0.2	0.3	...	0.8	0.9	1	N
$\kappa_5(t)$	1.4494	1.3553	1.2488	...	1.1916	1.1718	1.1306	20
	1.4412	1.3952	1.3312	...	1.1480	1.1182	1.0867	40
	1.4585	1.4068	1.3530	...	1.1485	1.1171	1.0869	80
	1.4630	**1.4157**	**1.3668**	...	**1.1490**	**1.1160**	**1.0872**	exact
$\kappa_6(t)$	1.9951	1.8954	1.7414	...	0.9140	0.6593	0.3681	20
	1.9948	1.9380	1.8300	...	0.8708	0.6051	0.3234	40
	1.9940	1.9496	1.8423	...	0.8701	0.6062	0.3329	80
	1.9937	**1.9418**	**1.8497**	...	**0.8731**	**0.6096**	**0.3396**	exact
$\kappa_7(t)$	2.2737	2.9683	3.7839	...	9.7888	11.4096	13.1782	20
	2.2758	2.9697	3.7821	...	9.7928	11.4133	13.1808	40
	2.2765	2.9700	3.7819	...	9.7942	11.4147	13.1821	80
	2.2772	**2.9708**	**3.7826**	...	**9.7951**	**11.4167**	**13.1853**	exact
$\kappa_8(t)$	1.3666	1.9433	2.6786	...	9.4391	11.5672	14.0063	20
	1.3677	1.9430	2.6755	...	9.4380	11.5675	14.0069	40
	1.3670	1.9427	2.6748	...	9.4371	11.5678	14.0072	80
	1.3664	**1.9410**	**2.6715**	...	**9.4377**	**11.5680**	**14.0080**	exact

In the inverse problem (14)–(21), we take the initial guesses for the vectors $\mathbf{l}, \mathbf{h}, \mathbf{b_1}$ and $\mathbf{b_2}$, as follows:

$$l^0(t_n) = l_0 = 1,\ h^0(t_n) = h_0 = 1,\ b_1^0(t_n) = b_1(0) = -1,\ b_2^0(t_n) = b_2(0) = -1,$$
$$n = \overline{1, N}, \quad (42)$$

by noting that the values of $b_1(0)$ and $b_2(0)$ are *a priori* obtainable from the system of equations (11)–(13). We take a mesh size with $M_1 = M_2 = 10$ and $N = 40$, which was found sufficiently dense to ensure that any finer mesh (such as $M_1 = M_2 = 20$ and $N = 80$) did not influence the stability and accuracy of the numerical solution.

For exact data, i.e. $p = 0$, although not illustrated, it is reported that the unregularized objective function (34) with $\lambda_i = 0$ for $i = \overline{1,4}$, is monotonically decreasing convergent to attain a very low stationary threshold. Furthermore, the rate of convergence increases with decreasing the time step. A good agreement between the analytical (40) and numerical solutions for the time-dependent functions $l(t)$, $h(t)$, $b_1(t)$ and $b_2(t)$ was observed with RMS(l) =1.9E-3, RMS(h) =3.7E-3, RMS(b_1) =0.1819 and RMS(b_2) =0.1522.

Next, the stability of the numerical solution is investigated when the data (35) is perturbed by a small amount $p = 0.01\%$ of noise. The objective function (34), without and with regularization is plotted in Figure 1, where rapid decreases to values of $O(10^{-22})$ and $O(10^{-2})$ are noticed in 42 and 15 iterations, respectively. The RMS values for $l(t)$, $h(t)$, $b_1(t)$ and $b_2(t)$ are presented in Figure 2. From this figure, it can be observed that RMS(l) and RMS(h) values are much lower than the RMS(b_i) for $i = 1, 2$, indicating that the free boundaries $l(t)$ and $h(t)$ are retrieved more accurately than the coefficients b_1 and b_2. Moreover, from Figure 2 it can be observed that in the case of no regularization, i.e. $\lambda_i = 0$, for $i = \overline{1,4}$, the RMS values settle to stationary levels after 10 to 20 iterations. The numerical results for $l(t)$, $h(t)$, $b_1(t)$ and $b_2(t)$ are depicted in Figure 3. Stable and accurate results are obtained for $l(t)$ and $h(t)$ by observing Figures 3(a) and 3(b), indicating that the inverse problem is stable in $l(t)$ and $h(t)$ and regularization is not necessary. However, if we do not impose regularization, unstable (highly oscillatory) behaviour for the coefficients $b_1(t)$ and $b_2(t)$, with RMS(b_1)=1.2885 and RMS(b_2)=1.1369, is obtained. Based on these observations, we choose $\lambda_1 = \lambda_2 = 0$, i.e. we do not penalise $\mathbf{l}$ and $\mathbf{h}$ in (34). In order to stabilise the terms $b_1(t)$ and $b_2(t)$, we have applied regularization with $\lambda_3 = \lambda_4 \in \{10^{-4}, 10^{-3}\}$, obtaining RMS($b_1$) $\in \{0.5644, 0.5724\}$ and RMS(b_2) $\in \{0.3702, 0.3729\}$, respectively. Clearly, the effect of $\lambda_3 = \lambda_4 > 0$ in drastically reducing the oscillatory unstable behaviour of $b_1(t)$ and $b_2(t)$ are noticed. Overall, Figures 3(c), 3(d) and Table 2 shows that the numerical results achieved with $\lambda_3 = \lambda_4 = 10^{-4}$ are stable and accurate. Finally, it is reported that the numerical solutions for $v(y_1, y_2, t)$ were found stable and accurate and, for brevity, they are not presented.

(a) (b)

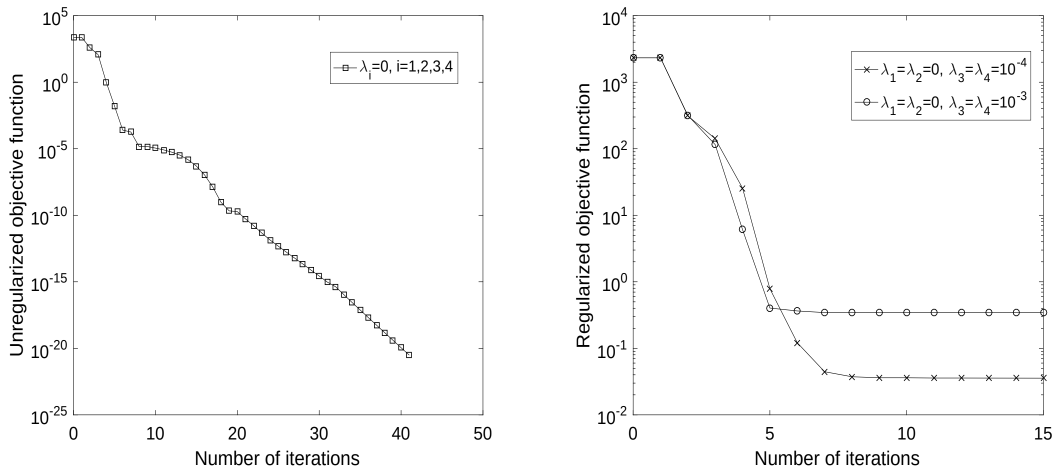
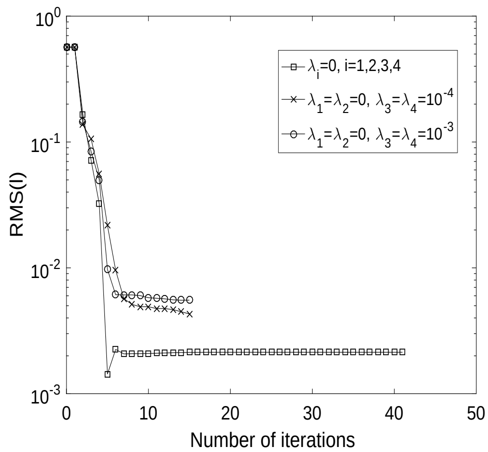


Figure 1: The objective function (34) versus the number of iterations: (a) without regularization, and (b) with regularization, for $p = 0.01\%$ noise.

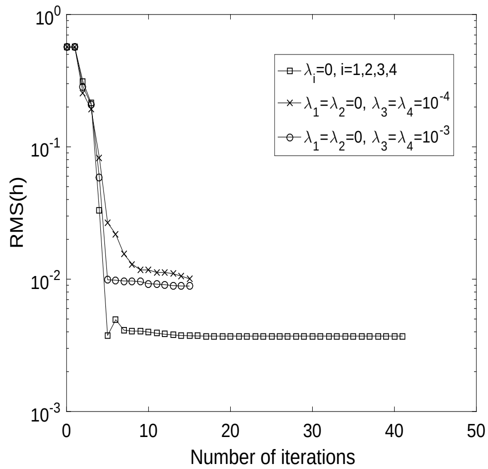
Table 2: The RMS at the stopping iteration numbers Iter for $p \in \{0, 0.01\%\}$ noise, without and with regularization.

p	λ_1	λ_2	λ_3	λ_4	RMS(l)	RMS(h)	RMS(b_1)	RMS(b_2)	Iter
0	0	0	0	0	0.0019	0.0037	0.1819	0.1522	37
0.01%	0	0	0	0	0.0021	0.0039	1.2885	1.1369	32
	0	0	10^{-5}	10^{-5}	0.0047	0.0098	0.9188	0.7562	16
	0	0	10^{-4}	10^{-4}	0.0040	0.0046	0.5644	0.3702	16
	0	0	10^{-3}	10^{-3}	0.0055	0.0089	0.5724	0.3729	16
	0	0	10^{-2}	10^{-2}	0.0133	0.0214	0.7433	0.3863	13
	0	0	10^{-1}	10^{-1}	0.0567	0.0870	0.9875	0.4542	17

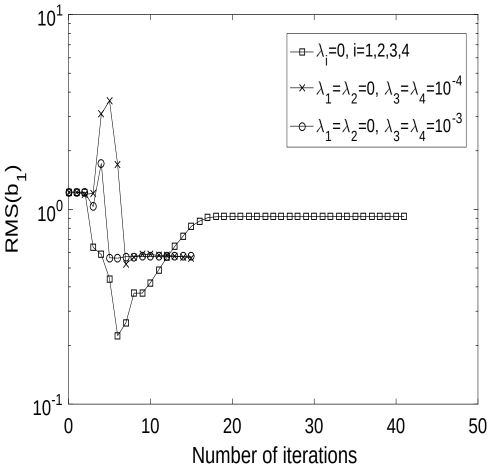
(a)



(b)



(c)



(d)

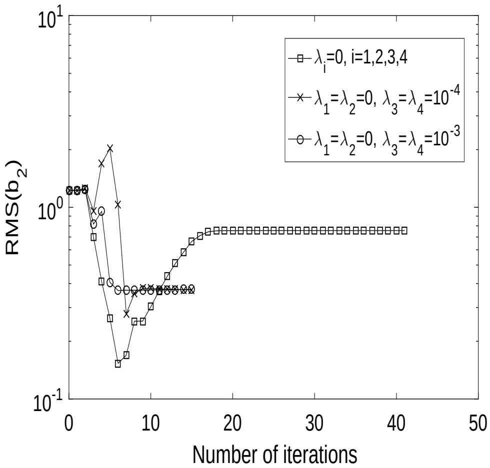


Figure 2: The RMS values: (a) RMS(l), (b) RMS(h), (c) RMS(b_1) and (d) RMS(b_2) versus the number of iterations, for $p = 0.01\%$ noise, without and with regularization.

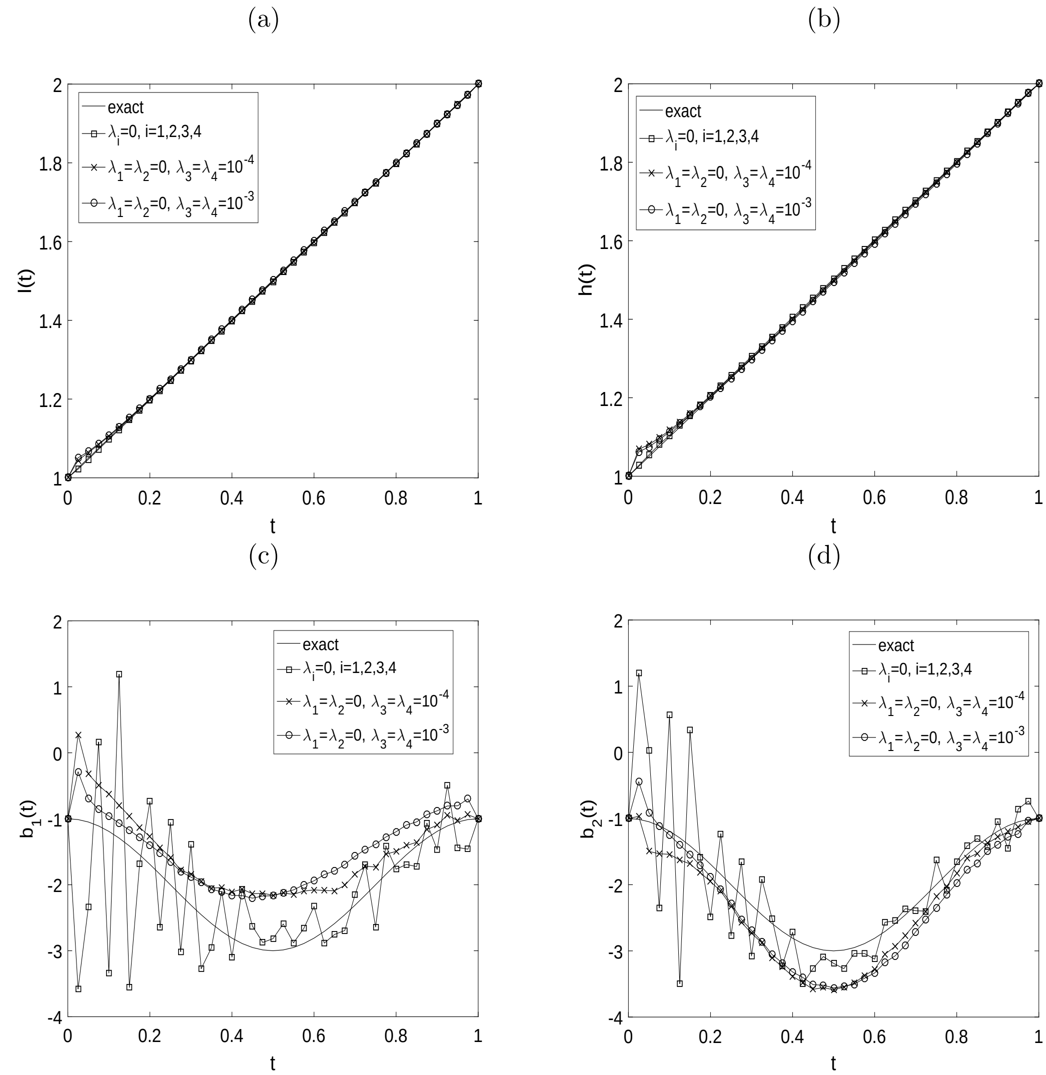


Figure 3: The exact (40) and numerical solutions for: (a) $l(t)$, (b) $h(t)$, (c) $b_1(t)$ and (d) $b_2(t)$, for $p = 0.01\%$ noise, without and with regularization.

6 Conclusions

In this study, an inverse free boundary problem concerning the determination of the time-dependent convection term $\underline{b}(t) = (b_1(t), b_2(t))$ and the free moving boundaries $l(t)$ and $h(t)$ along with the temperature $u(x_1, x_2, t)$ in the two-dimensional heat equation from over-specification conditions has been solved for the first time numerically. The study may be particularly useful not only to free boundary value problems in heat transfer and porous media, but also in problems related to clinical diagnose of cancer, [15]. The direct solver based on the ADE was employed. The inverse problem approach based on a nonlinear least-squares minimization problem using the MATLAB optimization subroutine was developed. The Tikhonov regularization has been employed in order to obtain stable and accurate solutions since the inverse problem is ill-posed in the convection coefficient with respect to noise in the nonlocal integral observations (5)-(8).

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