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Reconstruction of Timewise Dependent Coefficient and Free Boundary in Nonlocal Diffusion Equation with Stefan and Heat Flux as Overdetermination Conditions

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Abstract

The problem of reconstruction of a timewise dependent coefficient and free boundary at once in a nonlocal diffusion equation under Stefan and heat Flux as nonlocal overdetermination conditions have been considered. A Crank–Nicolson finite difference method (FDM) combined with the trapezoidal rule quadrature is used for the direct problem. While the inverse problem is reformulated as a nonlinear regularized least-square optimization problem with simple bound and solved efficiently by MATLAB subroutine *lsqnonlin* from the optimization toolbox. Since the problem under investigation is generally ill-posed, a small error in the input data leads to a huge error in the output, then Tikhonov's regularization technique is applied to obtain regularized stable results.

Keywords: Inverse problem; Free boundary; Nonlocal diffusion equation; Stefan condition; Implicit finite difference scheme; Tikhonov technique; Stability analysis.

إعادة بناء معامل يعتمد على الزمن مع حدود حرة معتمدة في معادلة الانتشار الغير محلية مع شرط ستيفان و شرط تدفق الحرارة الاضافي

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الخلاصة:

تم النظر في مشكلة إعادة بناء معامل يعتمد على الزمن مع حدود حرة بنفس الوقت في معادلة الانتشار غير المحلية تحت شرط Stefan وشرط تدفق الحرارة كشروط غير محلية. تم استخدام طريقة للفروقات المنتهية (FDM) مع مخطط Nicolson–Crank جنبًا إلى جنب مع trapezoidal rule quadrature لحل المشكلة المباشرة. بينما ، تم إعادة صياغة المشكلة العكسية كمسألة امثلية غير خطية من نوع اصغر التربيعات وحلها بكفاءة بواسطة روتين lsqnonlin من MATLAB. نظرًا لأن المشكلة هي معتلة بشكل عام ، فان اي خطأ صغير في بيانات الإدخال يؤدي إلى خطأ كبير في الإخراج ، لذلك تم تطبيق تقنية تنظيم Tikhonovللحصول على نتائج مستقرة ومنتظمة.

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1. Introduction

The inverse problems in a free domain (so called Stefan problems) arise in a variety of physical applications involving diffusion, heat transfer (thawing or freezing), and deformable porous medium problems where solid displacement is driven by diffusion. The history of Stefan's problems and their traditional solutions are thoroughly described in the monographs by [1, 2, 3]. The goal of the inverse Stefan problem is to either infer unknown thermo physical parameters or to establish an initial condition or a boundary condition using additional data, such as measurements of the temperature distribution at certain time instants or the location of the moving boundary interface. Since these inverse Stefan-type problems are typically ill-posed, regularization techniques are required to produce reliable numerical solutions. By"ill-posed", we mean that the solution does not rely on the input data continuously. Numerous direct and inverse Stefan problems have been solved using various numerical techniques. Adil and Hussein in [4] discussed the numerical solution for the Stefan's two-sided free boundary problem by using (FDM), while Kumar, Singh, et. al, [5] had applied the shifted Chebyshev tau method was used to solve Stefan's problem one-sided.

The numerical solution of the inverse problem was discussed by several authors just to mention only a few; in [6, 7, 8] they used optimization methods (Gauss-Newton, simulated annealing, genetic algorithms, Krylov Subspace and Quasi-Newton) to find solutions to nonlinear inverse problems. A relaxation factor optimization technique based on Newton Raphson's method to find solutions to one- and the two-dimensional transient nonlinear inverse was studied by John Crank [9]. Whilst, regularized Levenberg–Marquardt method was used in [10, 11, 12]. Also, in [13, 14] they investigated the application of Haar wavelet method to solve some inverse problems and LingDe, and Vasil'ev in [15] studied a new conjugate gradient method for two-dimensional space-dependent heat source problem.

One of the most widely used methods for solving nonlinear inverse problems is the least-squares minimization method, and it has been used by many authors. In [16, 17, 18] it was used to solve the time dependent parabolic heat inverse problem in one- and two-dimensions and the same method used to solve the nonlinear one-dimensional diffusion problem involves the partial differential equation under various boundary conditions and overdetermination conditions in [19, 20, 21, 22] to find the thermal conductivity $a(\tau)$ and in [23, 24] to find perfusion coefficient $b(\tau)$ in addition to $a(\tau)$.

The inverse problem under investigation in this work has already been shown to be uniquely solvable by M.I. Ivanchov [25], although, no numerical attempt for identification has been made so far; as a result, the main aim of this work is to the numerical realization of such problem. The novelty of the current study is the creation of FDM scheme combined with an optimization method for solving this nonlinear inverse problem to the nonlocal diffusion equation in a free boundary domain.

The following is the paper's structure: Section 2 is devoted to the mathematical formalism of the inverse problem. In section 3, the finite difference scheme is given to obtain the numerical solution for the direct problem with the numerical test example was provided. Whilst, in section 4, the numerical approach for solving inverse problems is given which is based on Tikhonov's technique to find a regularized solution. In section 5, numerical results are displayed and discussed. In the final section, the conclusions of this paper are given.

2. Mathematical description

Consider the one-dimensional nonlocal diffusion equation in one-side free boundary domain:

$$u_\tau(x,\tau) = a\left(\int_0^{k(\tau)} u(x,\tau)dx\right)u_{xx}(x,\tau) + f(x,\tau), \quad (x,\tau) \in \Omega_T, \tag{1}$$

under the initial condition

$$u(x,0) = \varphi(x), \qquad x \in [0, k(0)], \tag{2}$$

and the non-homogenous Dirichlet boundary conditions

$$u(0,\tau) = \xi_1(\tau), \quad u(k(\tau),\tau) = \xi_2(\tau), \quad \tau \in [0,T], \tag{3}$$

and the additional extra information (an integral and heat flux) condition,

$$a\left(\int_0^{k(\tau)} u(x,\tau)dx\right)u_x(0,\tau) = \xi_3(\tau), \qquad \tau \in [0,T], \tag{4}$$

and the Stefan condition

$$k'(\tau) = -u_x(k(\tau),\tau) + \xi_4(\tau), \qquad \tau \in [0,T], \tag{5}$$

where $\Omega_T = \{(x,\tau): 0 < x < k(\tau), 0 < \tau < T\}, k = k(\tau)$, is a free boundary and $s = \int_0^{k(\tau)} u(x,\tau)dx$, $a(s) > 0$, is the thermal conductivity which should be determined. Also, $k(0) = k_0 > 0$ is given .

Using Landau transformation $y = \frac{x}{k(\tau)}$ the above equations will transform into the following equations

$$v_\tau = \frac{1}{k^2(\tau)} a\left(k(\tau)\int_0^1 v(y,\tau)dy\right)v_{yy} + \frac{yk'(\tau)}{k(\tau)}v_y + f(yk(\tau),\tau), \ \ (y,\tau) \in Q_T, \tag{6}$$

$$v(y,0) = \varphi(yk), \qquad y \in [0,1], \tag{7}$$

$$v(0,\tau) = \xi_1(\tau), \qquad v(1,\tau) = \xi_2(\tau), \quad \tau \in [0,T], , \tag{8}$$

and the nonlocal overdetermination conditions are:

$$a\left(k(\tau)\int_0^1 v(y,\tau)dy\right)v_y(0,\tau) = k(\tau)\xi_3(\tau), \quad \tau \in [0,T], \tag{9}$$

$$k'(\tau) = -\frac{v_y(1,\tau)}{k(\tau)} + \xi_4(\tau), \quad k(0) = k_{0,} \qquad \tau \in [0,T]. \tag{10}$$

Where the transformed temperature is $v(y,\tau) := u(yk(\tau),\tau)$, $s = k(\tau)\int_0^1 v(y,\tau)dy$ and the fixed domain $Q_T = \{(y,\tau): 0 < y < 1,\ 0 < \tau < T\}$.
In equations (1)-(5) or (6)-(10), the functions $f(yk(\tau),\tau), \varphi(yk_0)$, $\xi_i(\tau), i = 1,2,3,4$ are given, while $a(s) > 0$, $k(\tau) > 0$ and the temperature $u(x,\tau\ )$ are unspecified.

If the coefficient $a(s)$ and the free boundary k are known then we have the direct problem (1)-(3) or (6)-(8) which can represent a crucial mathematical model. For instance, where u is the temperature the measurements are done using a local average rather than a point estimate.
Another application for the undergoing model is if u represents population density. In this case of a population migration, such as that of bacteria in a container, it is obvious that $a = a\left(\int_{\bar{\Omega}} u(x,\tau)dx\right)$ i.e., the migration velocity is determined by the total population in a subdomain. Also, if one wants to represent animals that have a proclivity to flee (attracted) crowded zones, a sensible assumption would be that an is growing (decreasing) function of its argument respectively, [26,27]. The existence and uniqueness of theorems for the solution of the inverse problem have been established by [25], and stated as follows;

Theorem 1 (Existence of the inverse problem solution)

Let the following conditions hold:

E1) $f \in C^{1,0}([0,\infty) \times [0,T]), \varphi \in C^1[0,k_0], \xi_i \in C^1[0,T], i = 1,2,\ \xi_j \in C[0,T],\ j = 3,4.$

E2) $f(x,\tau) \geq 0\ for\ (x,\tau) \in ([0,\infty) \times [0,T]), \varphi'(x) > 0,\ for\ x \in [0,k_0], \xi_2(\tau) < 0,$

$$\xi_3(\tau) > 0, \qquad \xi_2(\tau)\xi_4(\tau) - \xi_3(\tau) > 0, \qquad for\ \ \tau \in (0,T];$$

E3) (Compatibility conditions), $\varphi(0) = \xi_1(0)$, $\varphi(k_0) = \xi_2(0)$.

Then there exists a number $T_0 \in [0,T]$ such that the triplet $(k,a,v) \in C^1[0,T_0] \times C[0,S] \times C^{2,1}(\ Q_{T_0}) \cap C^{1,0}(\bar{Q}_{T_0})$, satisfied the equations (6)-(10) exist and $a(s) > 0,\ k(\tau) > 0$, where $\tau\ \in [0,T_0],\ s \in [0,S]$ and S, T_0 determined by input data.

Theorem 2 (Uniqueness of the inverse problem solution)

Suppose

$$f \in C^{1,0}([0,\infty) \times [0,T]), \varphi \in C^2[0,k_0]\ and\ \xi_3 \neq 0, \qquad for\ \tau \in (0,T],$$

then the equations (6)-(10) have a unique solution.

3. FDM scheme for direct (forward) problem

In this section, we are going to solve the direct problem, i.e. when unknown $k(\tau)$ and $a(s)$ are assumed to be given. In order to solve this problem, FDM is used for finding the solutions of the nonlocal problem given by equations (6)-(10). We divide the domain Q_T into $\mathrm{M} \times \mathrm{N}$ mesh with a spatial step size of $\Delta \mathrm{y} = \frac{1}{\mathrm{M}}$, and the time step size of $\Delta\tau = \frac{\mathrm{T}}{N}$, where M and N are given positive integers. The grid points are given by

$$y_i = i\Delta y, \qquad i = \overline{0,M},$$
$$\tau_j = j\Delta\tau\,, \qquad j = \overline{0,N},$$

we denote the discretized form of the quantities as follows; $v(y_i,\tau_j) := v_{i,j}$,

$$a\left(k(\tau_j)\int_0^1 v(y_i,\tau_j)dy\right) \coloneqq a(s_j),$$

$f(y_i,\tau_j) := f_{i,j}$ and $\varphi(x_i) := \varphi_i$ for $i = \overline{0,M}$, and $j = \overline{0,N}$. Then, by developing the Crank–Nicolson FDM and using the trapezoidal rule quadrature for approximation of the integration part, the discretizes nonlocal diffusion equation (6) which can be obtained as;

$$\frac{v_{i,j+1} - v_{i,j}}{\Delta\tau} = \frac{1}{2}(G_{i,j} + G_{i,j+1}), \qquad i = \overline{0,M}, j = \overline{0,N}, \tag{11}$$

where,

$$G_{i,j} = \frac{a(I_j)}{(k_j)^2}\left(\frac{v_{i+1,j} - 2v_{i,j} + v_{i-1,j}}{(\Delta y)^2}\right) + \frac{y_i k'_j}{k_j}\left[\frac{v_{i+1,j} - v_{i-1,j}}{2\Delta y}\right] + f_{i,j},$$
$$i = \overline{1,M-1}, j = \overline{0,N}\,.$$

We simplify the equation (11), so we get

$$-\left[a(I_{j+1})\frac{\Delta\tau}{2(\Delta y k_{j+1})^2} - \frac{y_i\Delta\tau k'_{j+1}}{4\Delta y k_{j+1}}\right]v_{i-1,j+1} + \left[1 + 2a(I_{j+1})\frac{\Delta\tau}{2(\Delta y k_{j+1})^2}\right]v_{i,j+1}$$
$$-\left[a(I_{j+1})\frac{\Delta\tau}{2(\Delta y k_{j+1})^2} + \frac{y_i\Delta\tau k'_{j+1}}{4\Delta y k_{j+1}}\right]v_{i+1,j+1} = \left[a(I_j)\frac{\Delta\tau}{2(\Delta y k_j)^2} - \frac{y_i\Delta\tau k'_j}{4\Delta y k_j}\right]v_{i-1,j}$$
$$\left[1 - 2a(I_j)\frac{\Delta\tau}{2(\Delta y k_j)^2}\right]v_{i,j} + \left[a(I_j\,)\frac{\Delta\tau}{2(\Delta y k_j)^2} + \frac{y_i\Delta\tau k'_j}{4\Delta y k_j}\right]v_{i+1,j} + \frac{\Delta\tau}{2}(f_{i,j} + f_{i,j+1})\,,$$

suppose that,

$$A_{i,j} = a(I_j)\frac{\Delta\tau}{2(\Delta y k_j)^2} - \frac{y_i \Delta\tau k_j'}{4\Delta y k_j},$$
$$B_j = a(I_j)\frac{\Delta\tau}{2(\Delta y k_j)^2},$$
$$C_{i,j} = a(I_j)\frac{\Delta\tau}{2(\Delta y k_j)^2} + \frac{y_i \Delta\tau k_j'}{4\Delta y k_j},$$

and,

$$I_j = \frac{k_j}{2N}\left(v_{0,j} + v_{M,j} + 2\sum_{i=1}^{M-1} v_{i,j}\right).$$

Then equation (6) can be written in difference equation form as follows

$$-A_{i,j+1}v_{i-1,j+1} + [1 + 2B_{j+1}]v_{i,j+1} - C_{i,j+1}v_{i+1,j+1} = A_{i,j}v_{i-1,j} + [1 - 2B_j]v_{i,j} + C_{i,j}v_{i+1,j} + \frac{\Delta\tau}{2}(f_{i,j} + f_{i,j+1}). \quad (12)$$

The FDM discretizes equations (7)-(10) as,

$$v(y_i, 0) = v_{i,0} = \varphi(y_i k_0), \quad i = \overline{0, M} \quad (13)$$
$$v(0, \tau_j) = v_{0,j} = \xi_1(\tau_j), \quad v(1, \tau_j) = v_{M,j} = \xi_2(\tau_j) \ , j = \overline{0, N} \quad (14)$$

the discrete form of overdetermination conditions are given by;

$$\xi_3(\tau_j) = \frac{a(I_j)(4v_{1,j} - v_{2,j} - 3v_{0,j})}{2\Delta y k_j}, \quad j = \overline{0, N}, \quad (15)$$
$$\xi_4(\tau_j) = k_j' + \frac{(4v_{M-1,j} - v_{M-2,j} - 3v_{M,j})}{2\Delta y\, k_j}, \quad j = \overline{0, N}, \quad (16)$$

for each time step τ_j, equations (12), (13) and (14) can be written in matrix form as $L_{(M-1)\times(M-1)}V_{j+1} = P$, where

L=
$$\begin{bmatrix} 1+2B_{j+1} & -C_{1,j+1} & 0 & 0 & \cdots & & & 0 \\ -A_{2,j+1} & 1+2B_{j+1} & -C_{2,j+1} & 0 & 0 & \cdots & & 0 \\ 0 & -A_{3,j+1} & 1+2B_{j+1} & -C_{3,j+1} & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots & & & & \vdots \\ & & & & & & & 0 \\ 0 & 0 & \cdots & & 0 & -A_{M-2,j+1} & 1+2B_{j+1} & -C_{M-2,j+1} \\ 0 & 0 & \cdots & & & 0 & -A_{M-1,j+1} & 1+2B_{j+1} \end{bmatrix},$$

$$V_{j+1} = [v_{1,j+1},\ v_{2,j+1},\ \ldots, v_{M-2,j+1},\ v_{M-1,j+1}]^T,$$

$$P = \begin{bmatrix} A_{1,j+1}\xi_1(\tau_{j+1}) + A_{1,j}\xi_1(\tau_j) + [1 - 2B_j]v_{1,j} + C_{1,j}v_{2,j} + \frac{\Delta\tau}{2}(f_{1,j} + f_{1,j+1}) \\ A_{2,j}v_{1,j} + [1 - 2B_j]v_{2,j} + C_{2,j}v_{3,j} + \frac{\Delta\tau}{2}(f_{2,j} + f_{2,j+1}) \\ \vdots \\ A_{M-2,j}v_{M-3,j} + [1 - 2B_j]v_{M-2,j} + C_{M-2,j}v_{M-1,j} + \frac{\Delta\tau}{2}(f_{M-2,j} + f_{M-2,j+1}) \\ C_{M-1,j+1}\xi_2(\tau_j) + A_{M-1,j}v_{M-2,j} + [1 - 2B_j]v_{M-1,j} + C_{M-1,j}\xi_2(\tau_j) + \frac{\Delta\tau}{2}(f_{M-1,j} + f_{M-1,j+1}) \end{bmatrix}$$

In order to test the accuracy and stability of the direct problem, let us consider the case where the parameters $a(s), k(\tau), \varphi(x)$ *and* $f(y,\tau)$ are given. So we have a problem (1)-(3) and the input data are taken as follows:

Assume $l = T = 1$, for simplicity;
$k(\tau) = 1 + \tau, \quad \tau \in [0,1]$,
$a(s) = s = 1 + e^{\tau}(1+\tau) - cos(1+\tau)\,, \ \tau \in [0,1]$,
$\varphi(x) = 1 + \sin(x)\,, \ x \in [0,1+\tau]$
$f(x,\tau) = e^{\tau} + (1 + e^{\tau}(1+\tau) - cos(1+\tau))\, sin(x)\,, \ x \in [0,1+\tau], \ \tau \in [0,1]$,
and the true solution is

$$u(x,\tau) = e^{\tau} + sin(x), \tag{17}$$

using Landau transformation

$$y = \frac{x}{k(\tau)} = \frac{x}{1+\tau}$$

the transformed quantities will be as follows;

$$v(y,\tau) = e^{\tau} + sin\big((1+\tau)y\big), \qquad (y,\tau) \in Q_T, \tag{18}$$

$$f(y,\tau) = e^{\tau} + (1 + e^{\tau}(1+\tau) - cos(1+\tau))\, sin\big((1+\tau)y\big), \quad (y,\tau) \in Q_T.$$

Therefore, the input data will be as follows;

$$\varphi(y) = v(y,0) = 1 + \sin(y), \qquad y \in [0,1],$$

$$\xi_1(\tau) = v(0,\tau) = e^{\tau}, \qquad \tau \in [0,1],$$

$\xi_2(\tau) = v(1,\tau) = e^{\tau} + sin(1+\tau), \quad \tau \in [0,1]$.
The desired outputs are

$$\xi_3(\tau) = 1 + e^{\tau}(1+\tau) - co\,s(1+\tau)\,, \quad \tau \in [0,1], \tag{19}$$

$$\xi_4(\tau) = 1 + co\,s(1+\tau)\,, \qquad \tau \in [0,1], \tag{20}$$

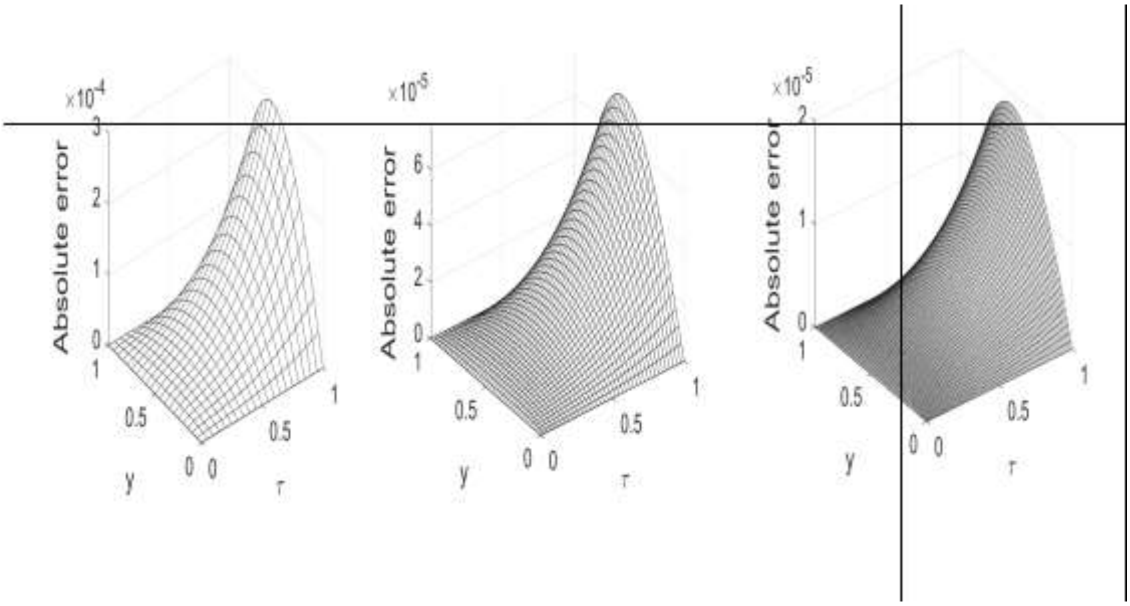

Figure 1: The graphs showing absolute errors for heat distribution for the direct problem (1)-(3), when mesh sizes $M = N \in \{20, 40,80\}$.

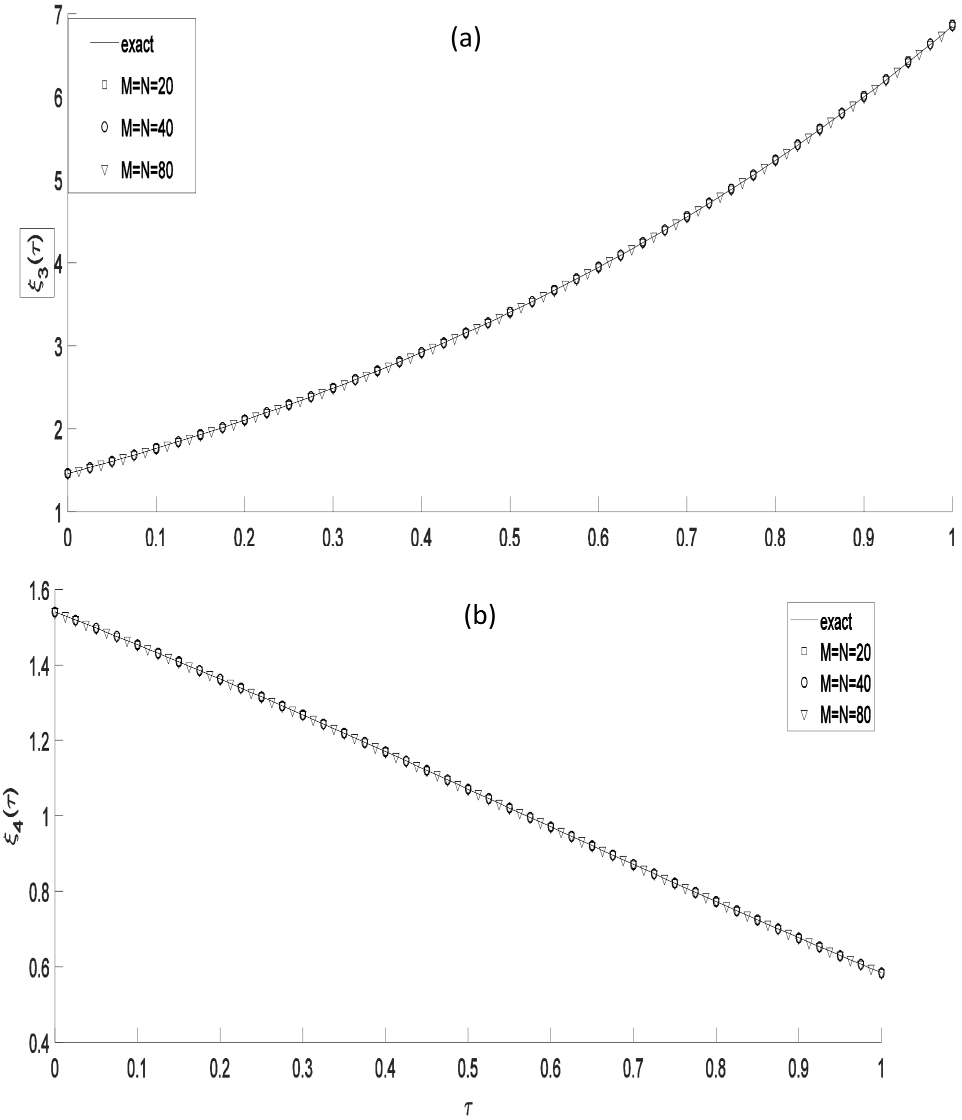

Figure 2: The exact and numerical values for desired output (a) $\xi_3(\tau)$, and (b) $\xi_4(\tau)$, with various mesh sizes $M = N \in \{20, 40, 80\}$.

Figure 1 presents the absolute error diagrams of interior domain points of heat distribution when sizes of mesh are taken as $M = N \in \{20, 40, 80\}$. Mesh independence has been attained, as well as numerical solution convergence toward exact ones and high agreement can be noticed. Figure 2, it is clear that as the number of discretization rises, the findings for $\xi_3(\tau)$ and $\xi_4(\tau)$ become more accurate showing a clear convergence.

4. Inverse Problem

For the nonlinear inverse problem (6)-(10), we aim to find numerical solutions for $a(s)$ and $k(\tau)$ simultaneously with transformed temperature distribution $v(y,\tau)$ satisfying the problem that is given by equations (6)-(10). At the initial time; i.e., at $\tau = 0$, we can use the input data to obtain initial values for a and k which will be described in the next subsection. Through the iterative process of solving the inverse problem, these numbers will be considered constant starting guesses. In order to tackle this challenge; the inverse problem is viewed as a nonlinear minimization problem. In other words, we want to keep the gap between observed data and numerically computed values as small as possible. We use the Tikhonov regularization approach to gain a stable and possible. We use the Tikhonov regularization approach to gain a stable and smooth solution because the problem under consideration is ill-posed. Overdetermination conditions (9) and (10) can be imposed to create the Tikhonov regularization functional as follows:

$$F(k,a)=\left\|\frac{a\left(k(\tau)\int_0^1 v(y,\tau)dy\right)v_y(0,\tau)}{k(\tau)}-\xi_3(\tau)\right\|^2+\left\|k'(\tau)+\frac{v_y(1,\tau)}{k(\tau)}-\xi_4(\tau)\right\|^2 +\beta_1\|k(\tau)\|^2+\beta_2\|a(\tau)\|^2, \quad (21)$$

where $\beta_i \geq 0, i=1,2$, are a regularization parameters and the norm is usually the $L^2[0,T]$. The discretization of (21) is

$$F(\underline{k},a)=\sum_{j=0}^{N}\left[\frac{a(s_j)v_y(0,\tau_j)}{k_j}-\xi_3(\tau_j)\right]^2+\sum_{j=0}^{N}\left[k'_j+\frac{v_y(1,\tau_j)}{k_j}-\xi_4(\tau_j)\right]^2+\beta_1\sum_{j=1}^{N}k_j^2 +\beta_2\sum_{j=1}^{N}a_j^2. \quad (22)$$

The unregularized case, i.e., $\beta_1=\beta_2=0$, produces the regular nonlinear least-squares functional, which is inherently unstable when dealing with noisy data. The MATLAB toolbox function *lsqnonlin* is used to minimize F under the physically required constraints $k>0,\ a>0$ and does not need the user to provide the gradient of the objective functional (22), see [28] for more details. The subroutine *lsqnonlin* seeks to determine the minimum of a scalar function of many variables; this is known as constrained nonlinear optimization. We take the parameters of the subroutine as follows:

• The maximum number of iterations (MaxIter) $=10^4\times$ N.
• Solution tolerance (SolTOL) and objective function tolerance (FunTOL) $=10^{-10}$.

The inverse problem (1)-(5) was solved subject to both exact and noisy measurements (4) and (5). The noisy data is numerically simulated by adding random errors to model the reality situation as follows:

$$\xi_i^{\epsilon_i}(\tau_j)=\xi_i(\tau_j)+\epsilon_i, \qquad i=1,2, \qquad j=\overline{0,N} \quad (23)$$

where $\epsilon_i, i=1,2$ are random Gaussian normal distribution vectors with mean zero and standard deviations σ_1 and σ_2 that are given by

$$\sigma_i = p \times \max_{\tau\in[0,T]}|\xi_i(\tau)|; \qquad i=1,2, \quad (24)$$

where p is the percentage of noise. We use the MATLAB bulletin function *normrnd* to generate the random variables $\underline{\epsilon_i}=(\epsilon_{i,j})$ and $i=1,2,\ j=\overline{0,N}$ as follows:

$$\underline{\epsilon_i} = normrnd(0,\sigma_i,N), \qquad i=1,2 \quad (25)$$

4.1 Initial guess

As mentioned above, during the iterative process of solving the inverse problem, we need an initial guess to start with. These values for $a(0)$ and $k(0)$ can be computed from input data as follows;

Consider the nonlinear inverse problem (1)-(5) with unknown coefficient $a(s)$, the nonlocal overdetermination condition at $\tau=0$ we have :

$$a\left(\int_0^{k_0} u(x,0)dx\right)u_x(0,0) = a\left(\int_0^{k_0} \varphi(x)dx\right)\varphi'(0) = \xi_3(0). \tag{26}$$

Therefore, the initial guess

$$a(0) = a\left(\int_0^{k_0} \varphi(x)dx\right) = \frac{\xi_3(0)}{\varphi'(0)}, \tag{27}$$

$$k(0) = k_0, \tag{28}$$

provided that $\varphi'(0)$ did not vanish.

5. Results and discussion

We examine and evaluate the numerical calculation results using the FDM in connection with the Tikhonov regularization approach, as described in the previous section. The root mean squares errors (*rmse*) were utilized

$$rmse(k) = \sqrt{\frac{1}{N}\sum_{i=1}^{N}\left(k_i^{exact} - k_i^{numerical}\right)^2}. \tag{29}$$

They were calculated in order to estimate the accuracy of the identified coefficient and similar expression for a can be used.

Now, consider the test example for the inverse problem (1)-(5) where the coefficients $a(s)$ and $k(\tau)$ are unknowns with the following input data and let $T = 1$ for simplicity:

$$\xi_1(\tau) = u(0,\tau) = \frac{\tau}{6} - 1, \quad \xi_2(\tau) = u(k(\tau),\tau) = \frac{\left(2-\frac{\tau}{6}\right)+\tau}{6} + cos\left(\left(3-\frac{\tau}{6}\right)\pi\right),$$

$$\xi_3(\tau) = a(s)u_x(0,\tau) = \frac{1}{60}\left(\frac{-11\tau^2}{432} + \frac{5\tau}{18} + \frac{sin\left(\frac{\pi\tau}{6}\right)}{\pi} + 0.533333\right),$$

$$\xi_4(\tau) = k'(\tau) + u_x(k(\tau),\tau) = \frac{-1}{6} + \pi sin\left(\left(\frac{\tau}{6} - 3\right)\pi\right)$$

$$f(x,\tau) = \frac{\pi^2}{60}\left(\frac{-11\tau^2}{432} + \frac{5\tau}{18} + \frac{sin\left(\frac{\pi\tau}{6}\right)}{\pi} + 0.533333\right)cos\big((1+x)\pi\big) + \frac{1}{6},$$

$$\varphi(x) = u(x,0) = \frac{x}{6} + cos\big((1+x)\pi\big)$$

Since a is a positive coefficient, this leads to $\xi_3(\tau) > 0$, and $\xi_2(\tau) < 0$. Also, one can check that the compatibility conditions $\varphi(0) = \xi_1(0)$, $\varphi(k_0) = \xi_2(0)$ and $\varphi'(x) > 0$ are satisfied too. If we select $a(s) = \frac{s+0.2}{10}, s \in [0,S]$,

where $S = max_{\tau\in[0,T]}\left|a\left(k(\tau)\int_0^1 v(y,\tau)dy\right)\right|$, then it will satisfy the condition $\xi_2(\tau)\xi_4(\tau) - \xi_3(\tau) > 0$, In addition, ξ_3 is non-vanishing function over the time interval. Therefore, the inverse problem (1)-(5) with the above input data has a unique solution. The exact solution for the inverse problem can be concluded as

$$u(x,\tau) = \frac{x+\tau}{6} + \cos\big((1+x)\pi\big), \quad (x,\tau) \in Q_T, \tag{30}$$

$$k(\tau) = \left(2 - \frac{\tau}{6}\right), \quad \tau \in (0,1). \tag{31}$$

The initial guess was $a_0 = 0.0533$ and $k_0 = 2$ given by equations (27) and (28), respectively.
The numerical investigation begins with the situation of no noise included, i.e., $p = 0$ in (24). The inverse problem was executed with various FDM mesh values, namely, $M = N \in \{10, 20, 40\}$, to study the convergence of the numerical solutions for *a(s)* and *k(τ)*, and the numerical findings were compared with the precise ones using root mean squares errors from equation (29), presented in Table 1 and Figure 3.

Table 1: The rmse(k) and rmse(a), without noise and regularization.

N=M	**10**	**20**	**40**
$\boldsymbol{rmse(k)}$	0.0097	0.0026	0.0014
$\boldsymbol{rmse(a)}$	0.0064	0.0022	0.0012

When there was no regularization, i.e. $\beta_i = 0, i = 1,2$ in (22). As seen in Figure 3 and more clearly in Table 1, the numerical outputs converge to precise values as N = M increases. The errors are calculated using the $rmse(k)$ and $rmse(a)$ functions in equation (29). Also, as $N = M$ rises, the number of iterations necessary to get the objective functional (22) below a very low value around $O(10^{-13})$ also increases, as illustrated in Figure 3(c) and Table 1 reveals that mesh independence obtained with high precision even with a coarse grid. As a result, we choose $N = M = 20$ as a suitably fine mesh in the rest of this section to ensure that additional refining has no substantial impact on the numerical findings' accuracy. Furthermore, the minimal number of variables results in a suitable amount of iterations and computing time for the objective function (22) to reach the minimum value.

Next, we perturb the measured data with $p \in \{1, 3,5,10\}\%$ noise as in equation (23). In the absence of regularization, the associated numerical results are presented in Figure 4(a)-(b). From this figure, it can be observed that the free boundary $k(\tau)$ did not affect by the inclusion of the noise. Whilst, the reconstructions of an unknown coefficient $a(s)$ becomes oscillatory and unstable as the noise level increases from 1% to 10%. This behavior is expected since the problem under investigation is ill-posed. Therefore, a sort of stabilization should be applied. Figure 4(c) shows the convergence of the unregularized objective function (22) which is plotted, versus the number of iterations, for various amounts of noise where the minimization achieved at each selection of noise at it takes about 20 iterations to reach minimum value around $O(10^{-18})$. Table 2 illustrates the *rmse* values for reconstructed functions $k(\tau)$ and $a(s)$ for various noise levels. From this table, it can be easily concluded that as the noise level increases the *rmse* values increases slightly.

Table 2: The *rmse(k)* and *rmse(a)* for different level noise and without regularization.

Noise level	$\boldsymbol{p = 1\%}$	$\boldsymbol{p = 3\%}$	$\boldsymbol{p = 5\%}$	$\boldsymbol{p = 10\%}$
$\boldsymbol{rmse(k)}$	0.0032	0.0044	0.0058	0.0094
$\boldsymbol{rmse(a)}$	0.0023	0.0027	0.0035	0.0056

Table 3: The *rmse(k)* and *rmse(a)* for the inverse problem when $p \in \{5\%, 10\%\}$ noise contaminated in the input data and various regularization parameter values selected.

Noise levels	$\beta_1=\beta_2$	10^{-6}	10^{-5}	10^{-4}	10^{-3}	10^{-2}	10^{-1}
5%	$rmse(k)$	0.0058	0.0057	0.0048	0.0186	0.0797	0.0797
	$rmse(a)$	0.0035	0.0035	0.0045	0.0470	0.0375	0.0375
10%	$rmse(k)$	0.0094	0.0093	0.0084	0.0198	0.0801	0.0811
	$rmse(a)$	0.0056	0.0057	0.0065	0.0483	0.0375	0.0391

As mentioned before, to restore stability some regularization should be applied. We applyTikhonov type regularization method by adding Tikhonov penalty term $(\beta_1\|k(\tau)\|^2 + \beta_2\|a(\tau)\|^2)$. The identified outputs are presented in Figure 6 (a)-(b). This figure and Figure 5(a)-(b) exhibit that the unregularized case, for unknown k is much more stable than a. Since this behavior is seen in [19, 24] due to the explicit appearance of a free boundary in (22). We apply equal values for $\beta_1 = \beta_2$ to the rest of our computations because the problem under investigation seems to be ill-posed solely in a. A variety of regularization parameters $\beta_1 = \beta_2 \in \{10^{-6}, 10^{-5}, \ldots, 10^{-1}\}$ is used to get a stable solution, for various noise level such as $p \in \{5, 10\}\%$. Figure 6(c) displays the convergent minimization of (22), for $p = 5\%$, the decreasing process was terminated because the allowed accuracy 10^{-10} has been reached. The associated numerical reconstructions plotted in Figure 6(a)-(b) and very good retrievals have been obtain for $\beta_1 = \beta_2 \in [10^{-5}, 10^{-4}]$, and $p \in \{5, 10\}\%$ noise. To justify the selections of regularization parameters, there are several methods such as the L-curve method by P. Hansen [29], Morozov's discrepancy principle [30], trial and error as suggested in [31]. We adopted the last technique which is based on selecting small values for the regularization parameter and gradually increasing it until the instabilities start to disappear.

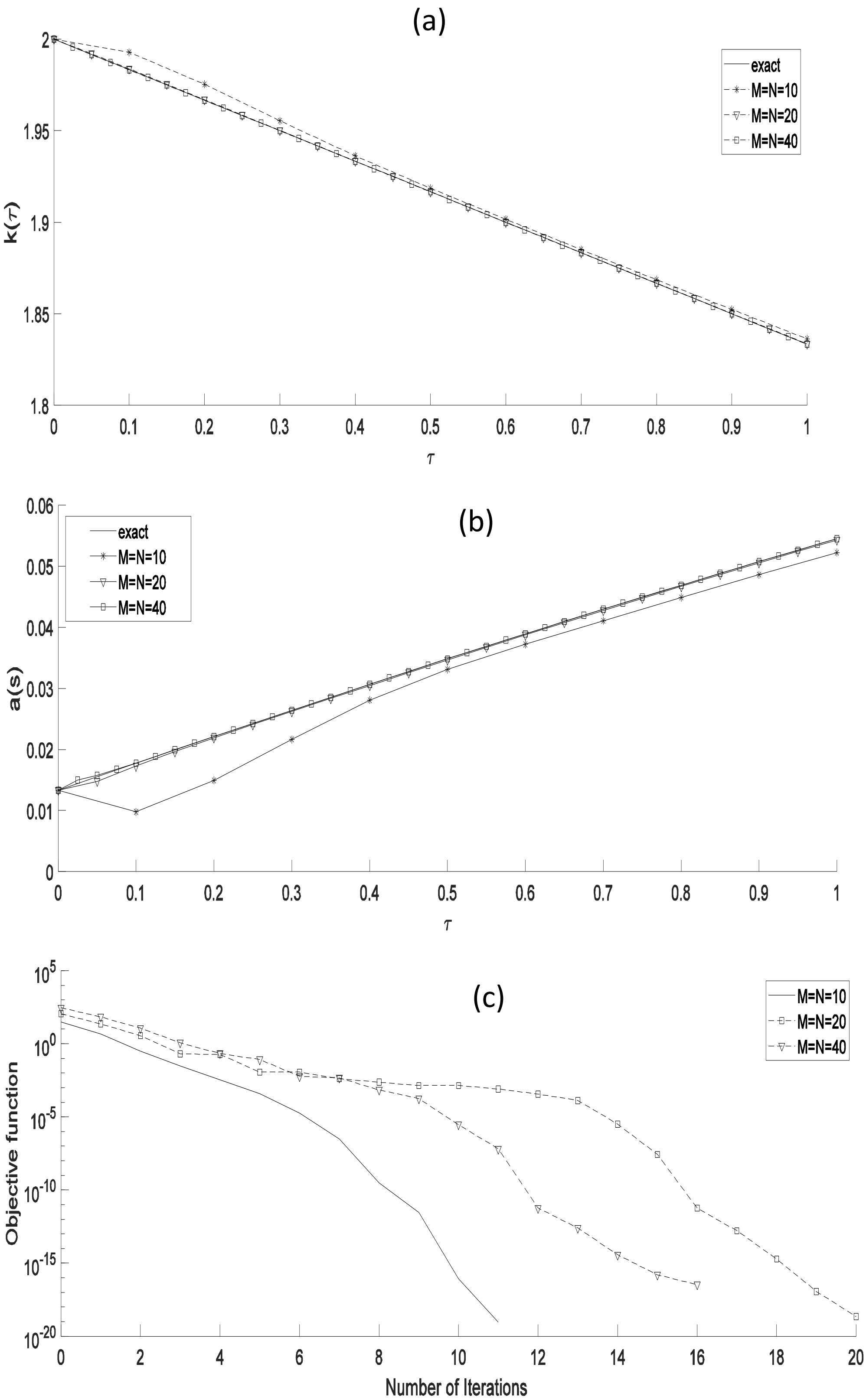

Figure 3: The functions(a) $k(\tau)$, (b) *a(s)* and (c) objective function (22), with noise free and without regularization,

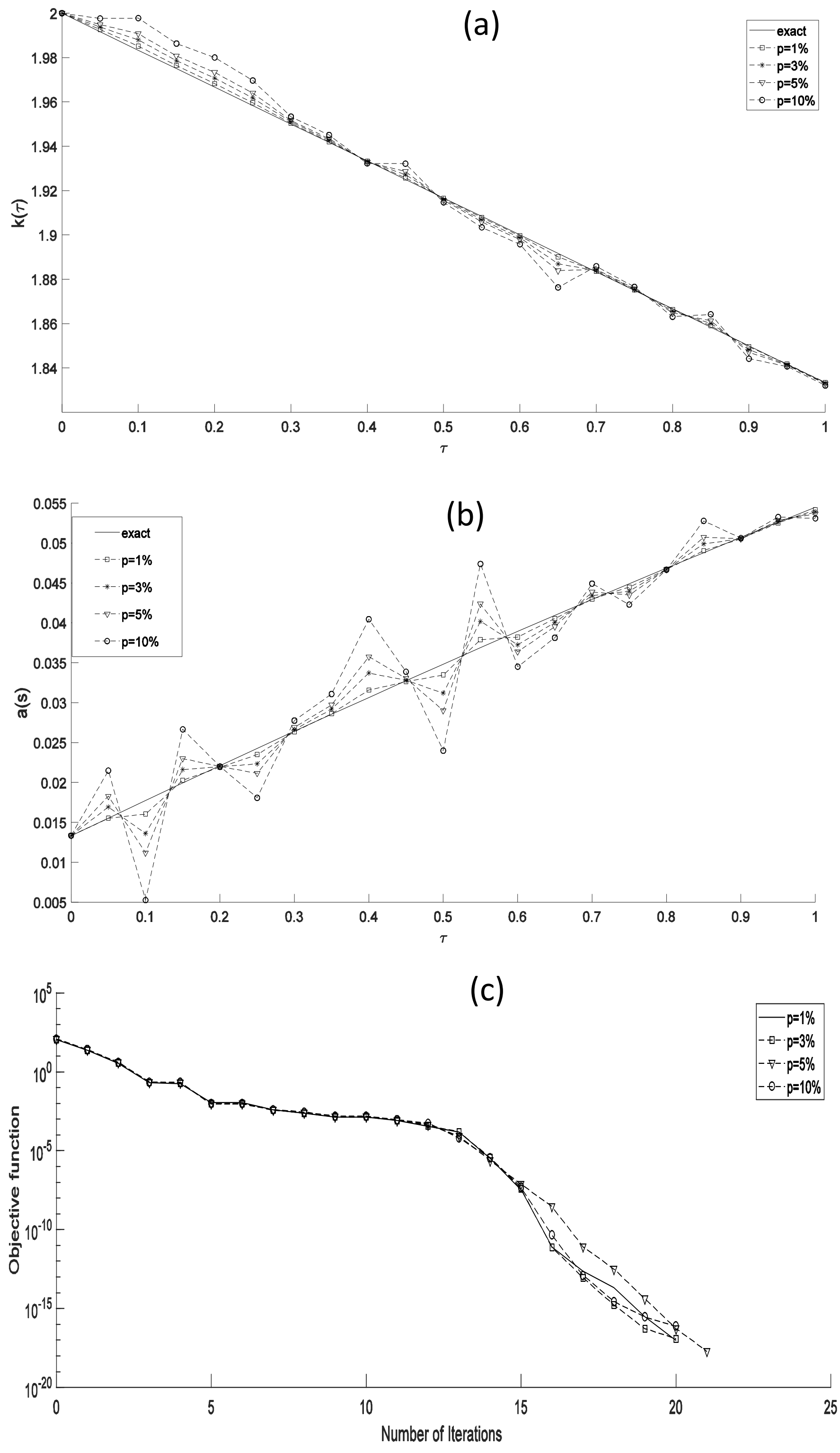

Figure 5: The reconstructions of (a) $k(\tau)$, (b) *a(s)* and (c) The objective function (22), for different noise level $p \in \{1, 3, 5, 10\}\%$ and no regularization.

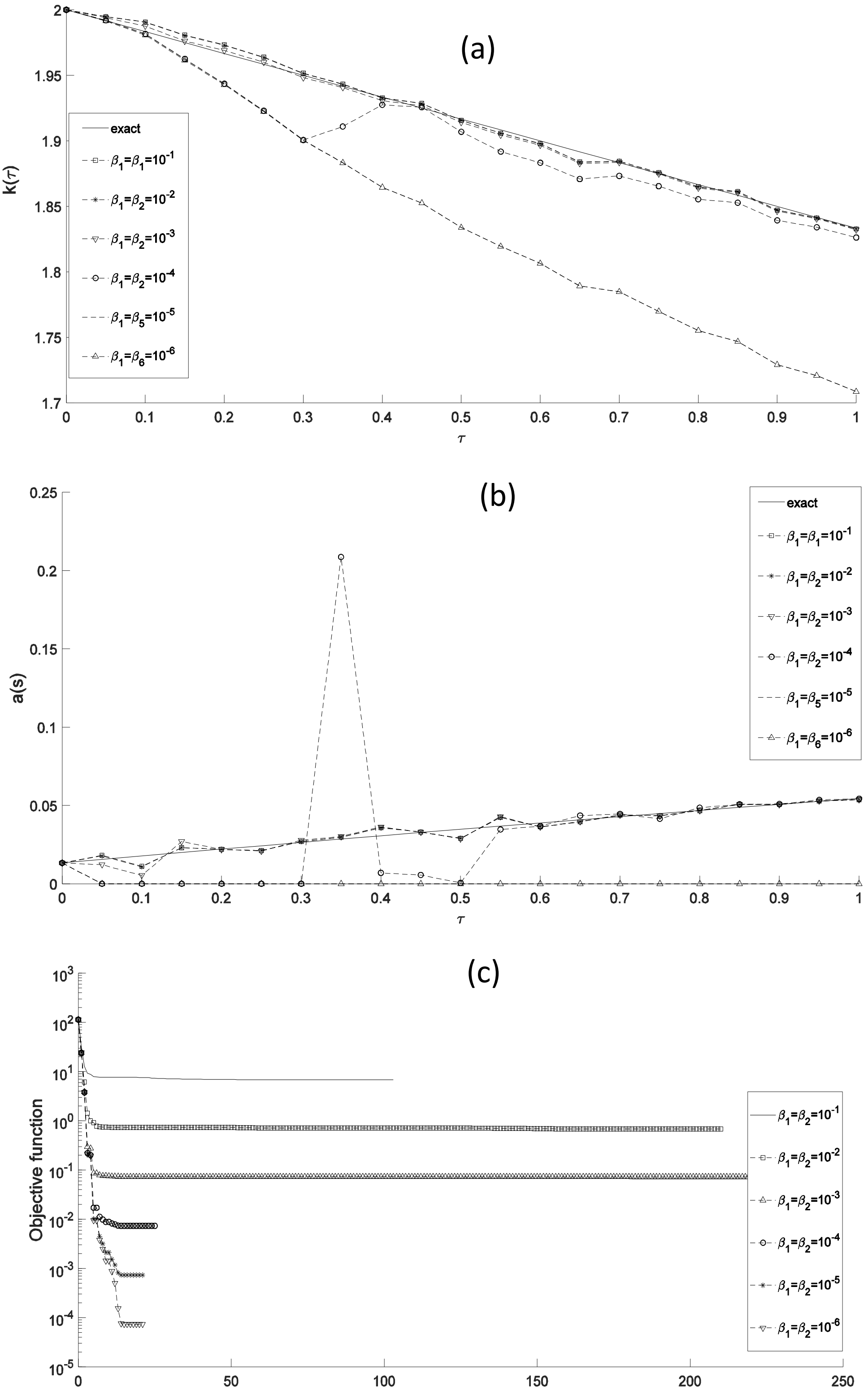

Figure 6: (a) $k(\tau)$, (b) *a(s)* and (c) The objective function (22), for $p = 5\%$ noise and $\beta_1 = \beta_2 \in \{10^{-1}, 10^{-2}, \ldots, 10^{-6}\}$.

In Figures 7, the transformed temperature $v(y, \tau)$ reconstructions are shown. In general, the addition of noise has no major effect on the temperature in terms of stability.

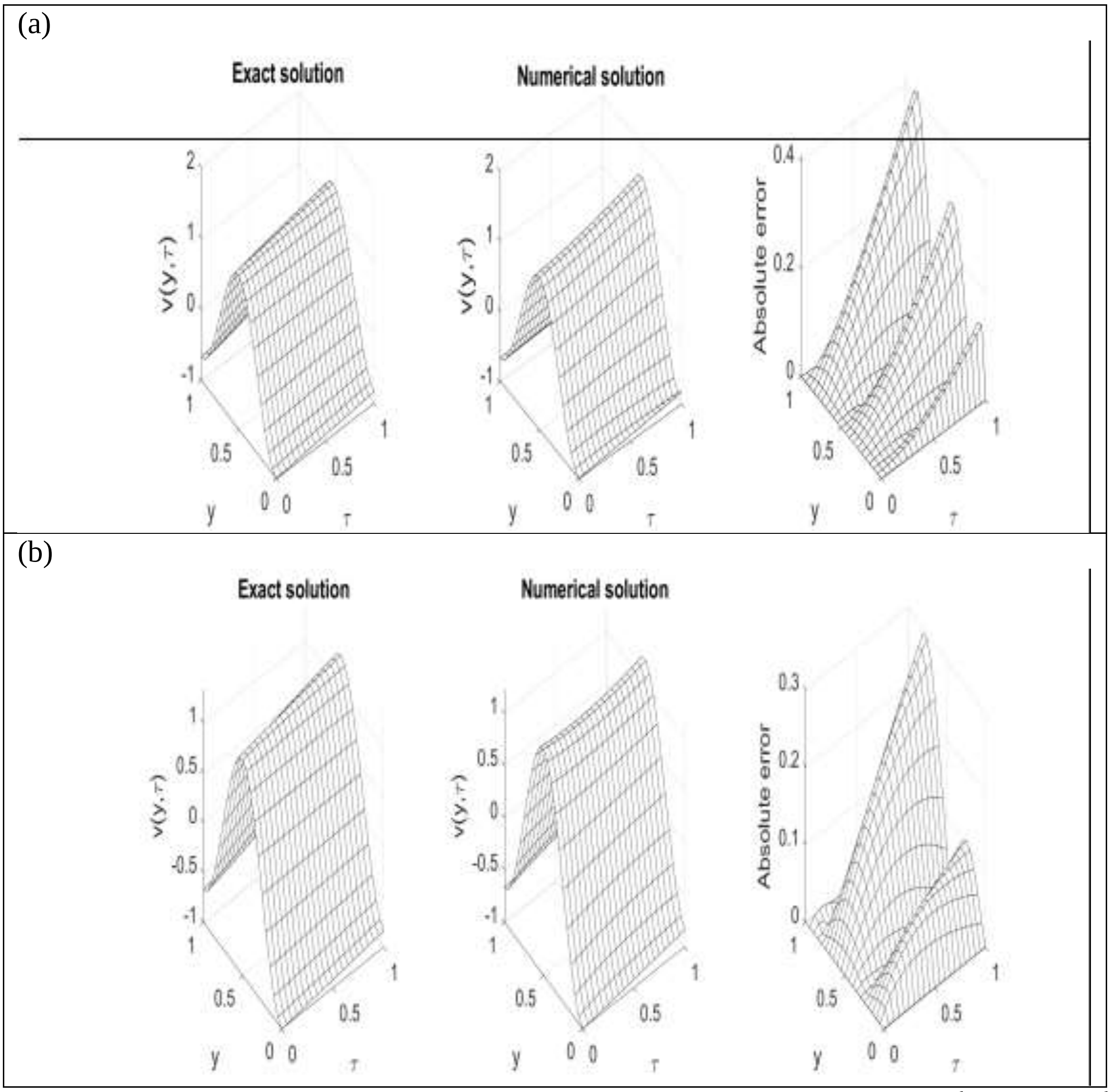

Figure 8: The exact and numerical temperatures $v(y,\tau)$, with (a) $\beta_1 = 10^{-6}, \beta_2 = 10^{-6}$, with $p = 5\%$ noise, (b) $\beta_1 = 10^{-5}, \beta_2 = 10^{-2}$, with $p = 10\%$ noise and the absolute error between them also calculated

6. Conclusions

In the nonlocal diffusion equation, with Stefan and heat flux acting as nonlocal additional conditions, the nonlinear inverse problem of reconstruction of the time-dependent thermal conductivity $a(s)$ and free boundary $k(\tau)$ have been studied numerically. The FDM scheme that is based on Crank-Nicolson has been developed to solve the forward (direct) problems and the trapezoidal quadrature rule is used to approximate the integral term. Whilst, the inverse problem was addressed iteratively using the MATLAB optimization toolbox routine *lsqnonlin*. The computational findings produced for both noisy and exact data have been analyzed and indicating that they are accurate and stable for various noise levels in presence of regularization with appropriate choice. Moreover, the results reveal that even with the inclusion of a high level of noise such as 10%, the free boundary and the temperature distributions do not affect by noise whilst the thermal coefficient part needs to be regularized via the Tikhonov penalty term added to the misfit functional. This technique can be extended/applied to more complicated inverse problems involving free/moving boundaries and will be a matter of future work.

References

[1] J. Crank. "*Free and moving boundary problems". Oxford University Press, USA*, 1984.
[2] M. James. "One-dimensional Stefan problems: an introduction", *Longman Sc. & Tech,* vol.31, 1987.
[3] I. Malyshev. "An inverse source problem for heat equation". *Journal of Mathematical Analysis and Applications,* vol.142, pp.206–218, 1989.
[4] Z. Adil and M.S. Hussein, "Numerical solution for two-sided Stefan problem". *Iraqi Journal of Science,* pp.444–452, 2020.
[5] A. Kumar, A. Kumar Singh, et al. "A Stefan problem with temperature and time-dependent thermal conductivity". *Journal of King Saud University-Science,* vol.32, no.1, pp.97– 101,2020.
[6] E. Haber, Uri M. Ascher, and D. Oldenburg. "On optimization techniques for solving nonlinear inverse problems". *Inverse problems,* vol.16, no. 5, pp.1263, 2000.
[7] J. A. Scales, M. L. Smith, and T. L. Fischer. "Global optimization methods for multimodal inverse problems". *Journal of Computational Physics,* vol.103, no.2, pp.258–268,1992.
[8] N. Ye, F. Roosta-Khorasani, and T. Cui. "Optimization methods for inverse problems". *In 2017 MATRIX Annals, Springer,* pp.121–140, 2019.
[9] M. Cui and Xiao-wei Duan. "A new inverse analysis method based on a relaxation factor optimization technique for solving transient nonlinear inverse heat conduction problems". *International Journal of Heat and Mass Transfer,* vol. 90, pp.491–498, 2015.
[10] Z. Fu, B. Han, and Y. Chen. "Levenberg–Marquardt method with general convex penalty for nonlinear inverse problems". *Journal of Computational and Applied Mathematics,* vol.404, pp.113771, 2022.
[11] Q. Jin. "On a regularized Levenberg–Marquardt method for solving nonlinear inverse problems". *Numerische Mathematik*, vol. 115, no. 2, pp. 229–259, 2010.
[12] J. Pujol. "The solution of nonlinear inverse problems and the Levenberg-Marquardt method". Geophysics, vol.72, no. 4, pp. W1–W16, 2007.
[13] M. Ahsan and I. Hussain. "Haar wavelets multi-resolution collocation analysis of unsteady inverse heat problems". *Inverse Problems in Science and Engineering,* vol. 27, no.11, pp.1498–1520, 2019.
[14] M. Ahsan, I. Hussain, and M. Ahmad. "A finite-difference and Haar wavelets hybrid collocation technique for non-linear inverse Cauchy problems". *Applied Mathematics in Science and Engineering,* vol.30, no.1, pp.121–140, 2022.
[15] LingDe Su and V.I. Vasil'ev. "Identification of spacewise dependent right-hand side in two dimensional parabolic equation". *In Journal of Physics: Conference Series,* vol.2092, pp.012-019. IOP Publishing, 2021.
[16] F. Anwer and M.S. Hussein. "Retrieval of time wise coefficients in the heat equation from nonlocal overdetermination conditions". *Iraqi Journal of Science,* vol.63, no.3, pp.1184– 1199, 2022.
[17] M.J. Huntul, M. S. Hussein, D. Lesnic, M.I. Ivanchov, and N. Kinash. "Reconstruction of an orthotropic thermal conductivity from nonlocal heat flux measurements". *International Journal of Mathematical Modeling and Numerical Optimization,* vol.10, no.1, pp.102– 122, 2019.
[18] M.J. Huntul and D. Lesnic. "An inverse problem of finding the time-dependent thermal conductivity from boundary data". *International Communications in Heat and Mass Transfer,* vol.85, pp.147–154, 2017.
[19] Z. Adil, M.S. Hussein, and D. Lesnic. "Determination of time-dependent coefficients in moving boundary problems under nonlocal and heat moment observations".

International Journal for Computational Methods in Engineering Science and Mechanics, vol. 22, no.6, pp. 500–513, 2021.

[20] M.S. Hussein and D. Lesnic. “Determination of the time-dependent thermal conductivity in the heat equation with spacewise dependent heat capacity”. vol.9045, pp.217–224, 2015.

[21] M.S. Hussein, D. Lesnic, and M.I. Ismailov. “An inverse problem of finding the time-dependent diffusion coefficient from an integral condition”. *Mathematical Methods in the Applied Sciences*, vol.39, no.5, pp.963–980, 2016.

[22] M. Qassim and M.S. Hussein. “Numerical solution to recover time-dependent coefficient and free boundary from nonlocal and Stefan type overdetermination conditions in heat equation”. *Iraqi Journal of Science,* vol.62, no. 3 pp. 950–960, 2021.

[23] M. S. Hussein and D. Lesnic. “Simultaneous determination of time and space dependent coefficients in a parabolic equation”. *Communications in Nonlinear Science and Numerical Simulation,* vol.33, no.4, pp.194–217, 2016.

[24] M.S. Hussein, D. Lesnic, M.I. Ivanchov, and H.A. Snitko. “Multiple time-dependent coefficient identification thermal problems with a free boundary”. *Applied numerical mathematics,* vol.99, pp.24–50, 2016.

[25] M.I. Ivanchov and G.A. Snitko. “Nonlocal inverse problem for the diffusion equation in the domain with free boundary”. *Bukovynian Mathematical Journal,* vol.77, pp.103-108, 2012.

[26] M. Chipot and B. Lovat. “On the asymptotic behaviour of some nonlocal problems”. *Positivity,* vol.3, no.1, pp.65–81, 1999.

[27] C. Michel and M. Lue. “Asymptotic behaviour of some nonlocal diffusion problems”. *Applicable Analysis*, vol.80, no.3-4, pp. 279–315, 2001.

[28] Mathworks. “Documentation optimization toolbox-least squares algorithms”. 2021.

[29] P. C. Hansen and D. P. O’Leary. “The use of the L-curve in the regularization of discrete ill-posed problems”. *SIAM journal on scientific computing,* vol.14, no.6, pp.1487–1503, 1993.

[30] T. Bonesky. “Morozov’s discrepancy principle and tikhonov-type functionals”. *Inverse Problems*, vol.25, no.1, pp.015015, 2008.

[31] B. H. Dennis, G. S. Dulikravich, and S. Yoshimura. “A finite element formulation for the determination of unknown boundary conditions for three-dimensional steady thermoelastic problems”. *J. Heat Transfer*, vol.126, no.1, pp.110–118, 2004.