Article:

Hussein, MS, Lesnic, D and Ivanchov, M (2013) Free boundary determination in nonlinear diffusion. East Asian journal on applied mathematics, 3 (4). 295 - 310. ISSN 2079-7362

https://doi.org/10.4208/eajam.100913.061113a

Free boundary determination in nonlinear diffusion

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Abstract
Free boundary problems with nonlinear diffusion occur in some applications concerning the solidification over a mould with dissimilar nonlinear thermal properties or, saturated/unsaturated absorption in the soil beneath a pond. In this paper, we consider a novel inverse problem of determining a free boundary from the mass/energy specification in a one-dimensional nonlinear diffusion. It turns out that this problem is well-posed and a stability estimate is established. Numerically, the problem is recast as a nonlinear least-squares minimization problem which is solved using the *lsqnonlin* routine from the MATLAB toolbox. Numerical results are presented and discussed showing that accurate and stable numerical solutions are achieved. For noisy data, the instability is manifested in the derivative of the moving free surface, but not in the free surface itself, or the concentration/temperature.

Keywords: Nonlinear diffusion; Free boundary problem; Finite-difference method.

1 Introduction

Driven by the demands from applications both in industry and other sciences, the field of inverse problem has undergone a tremendous development with in the last decades, where resent emphasis has been given for nonlinear inverse problems. In [2, 3], the authors investigated the problem of determining unknown coefficients for a nonlinear heat conduction problem together with temperature. While the problem of nonlinear diffusion with a free boundary was considered in [1], where the Stefan solidification problem was modelled as such. In addition, in [11] the authors developed a procedure to find an approximate stable solution to the unknown coefficient from over specification data based on the finite difference method combined with Tikhonov's regularization approach. In this work, we consider the problem of identifying the free boundary in a nonlinear diffusion problem.

This paper is organized as follows. In the next section, we give the formulation of the inverse problem under investigation. The numerical methods for solving the direct and inverse problems are described in Sections 3 and 4, respectively. Furthermore, the numerical results and discussion are given in Section 5 and finally, conclusions are presented in Section 6.

2 Mathematical formulation

In this section we consider the nonlinear one-dimensional diffusion equation which given by

$$\frac{\partial u}{\partial t}(x,t) = \frac{\partial}{\partial x}\left(a(u)\frac{\partial u}{\partial x}(x,t)\right) + f(x,t), \qquad (x,t) \in \Omega, \tag{1}$$

where the domain $\Omega = \{(x,t) : 0 < x < h(t), 0 < t < T < \infty\}$ with unknown free smooth boundary $x = h(t) > 0$. The initial condition is

$$u(x,0) = \phi(x), \qquad 0 \le x \le h(0) =: h_0, \tag{2}$$

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

$$u(0,t) = \mu_1(t), \qquad u(h(t),t) = \mu_2(t), \qquad 0 \le t \le T, \tag{3}$$

In order to determine the unknown boundary $h(t)$ for $t \in (0,T]$ we impose the over-determination condition of integral type

$$\int_0^{h(t)} u(x,t)dx = \mu_3(t), \qquad 0 \le t \le T, \tag{4}$$

which represents the specification of mass/energy of the diffusion system, see [4]. In the above, the functions $a > 0$, ϕ, μ_i, $i \in \{1,2,3\}$ and f are given. In (1), u represents the concentration/ temperature, f represent a source/sink, and a represents the diffusivity.

The pair of functions $(h(t), u(x,t)) \in C^1[0,T] \times C^{2,1}(\overline{\Omega})$ with $h > 0$ is said to be a solution of problem if fulfills the equations (1)–(4).

The mathematical model (1)–(4) has been considered in [6] where the following existence and uniqueness of solution theorems are proved.

Theorem 1. (Existence)
Assume that the following assumptions are fulfilled:

1. $\phi \in C^2[0,h_0]$, $\mu_i \in C^1[0,T]$, $i \in \{1,2,3\}$, $f \in C^{1,0}([0,H_1] \times [0,T])$, $a \in C^1[M_0,M_1]$;
2. $\phi(x) > 0$ *for* $x \in [0,h_0]$, $\mu_i > 0$ *for* $t \in [0,T]$, $i \in \{1,2,3\}$, $f(x,t) \ge 0$ *for* $(x,t) \in [0,H_1] \times [0,T]$, $a(s) \ge a_0 > 0$ *for* $s \in [M_0,M_1]$, *where* a_0 *is some given constant;*
3. $\mu_1(0) = \phi(0)$, $\quad \mu_2(0) = \phi(h_0)$, $\quad \int_0^{h_0} \phi(x)dx = \mu_3(0)$,
   $\mu_1'(0) = a(\mu_1(0))\phi''(0) + a'(\mu_1(0))\phi'^2(0) + f(0,0)$,
   $\mu_2'(0) = a(\mu_2(0))\phi''(h_0) + a'(\mu_2(0))\phi'^2(h_0) + \phi'(h_0)h'(0) + f(h_0,0)$.

Then the inverse problem (1)–(4) is locally solvable (in time).

Theorem 2. (Uniqueness)
Suppose that condition 2. of Theorem 1 and the following condition

$$a(s) \in C^1[M_0,M_1], \quad f(x,t) \in C^{1,0}([0,H_1] \times [0,T])$$

holds. Then a solution of the inverse problem (1)–(4) is unique.

In the above theorems, the constants H_1, M_0 and M_1 have the following meaning using the maximum principle [5] for the heat equation (1):

$$H_1 = \frac{1}{M_0} \max_{[0,T]} \mu_3(t), \quad M_0 = \min\{\min_{[0,h_0]} \phi(x), \ \min_{[0,T]} \mu_1(t), \ \min_{[0,T]} \mu_2(t)\},$$
$$M_1 = \max\{\max_{[0,h_0]} \phi(x), \ \max_{[0,T]} \mu_1(t), \ \max_{[0,T]} \mu_2(t), \ \max_{[0,H_1]\times[0,T]} f(x,t)\}.$$

We can also derive a formula for $h'(0)$ by differentiating equation (4) with time, and using equations (1)–(3) to obtain

$$h'(0) = \frac{\mu_3'(0) - a(\mu_2(0))\phi'(h_0) + a(\mu_1(0))\phi'(0) - \int_0^{h_0} f(x,0)dx}{\mu_2(0)}. \tag{5}$$

We perform the change of variable $y = x/h(t)$ to reduce the problem (1)–(4) to the following equivalent inverse problem in a rectangular domain for the unknowns $h(t)$ and $v(y,t) := u(yh(t),t)$, [6]:

$$\frac{\partial v}{\partial t}(y,t) = \frac{1}{h^2(t)} \frac{\partial}{\partial y}\left(a(v)\frac{\partial v}{\partial y}(y,t)\right) + \frac{yh'(t)}{h(t)}\frac{\partial v}{\partial y}(y,t) + f(yh(t),t), \qquad (y,t) \in Q \tag{6}$$

where $Q = \{(y,t) : 0 < y < 1, 0 < t < T\}$. The initial condition is

$$v(y,0) = \phi(h_0 y), \qquad 0 \le y \le 1, \tag{7}$$

and the boundary and over-determination conditions are

$$v(0,t) = \mu_1(t), \qquad v(1,t) = \mu_2(t), \qquad 0 \le t \le T, \tag{8}$$
$$h(t)\int_0^1 v(y,t)dy = \mu_3(t), \qquad 0 \le t \le T. \tag{9}$$

At the end of this section we establish the continuous dependence of the free boundary $h(t)$ on the input energy data (4).

Theorem 3. (Stability)
Suppose that the conditions of Theorem 1 are satisfied. Let μ_3 and $\tilde{\mu}_3$ be two data (4) and let $(h(t), u(x,t))$ and $(\tilde{h}(t), \tilde{u}(x,t))$ be the corresponding solutions of the inverse problem (1)–(4). Then there is a positive constant C such that the following stability estimate holds:

$$\|h - \tilde{h}\|_{C^1[0,T]} + \|v - \tilde{v}\|_{C^{1,0}(\overline{\Omega})} \le C\|\mu_3 - \tilde{\mu_3}\|_{C^1[0,T]}, \tag{10}$$

where

$$v(y,t) = u(yh(t),t), \quad \tilde{v}(y,t) = \tilde{u}(y\tilde{h}(t),t), \quad (y,t) \in Q. \tag{11}$$

Proof. In order to establish the stability estimate (10) we follow the proof of uniqueness of solution given in [6]. Denote $p(t) := h(t) - \tilde{h}(t)$, $q(t) := h'(t) - \tilde{h}'(t)$, $W(y,t) := v(y,t) - \tilde{v}(y,t)$ and $\Delta\mu_3(t) := \mu_3(t) - \tilde{\mu_3}(t)$. First from (9) one obtains that

$$\mu_3(t) = h(t)\int_0^1 v(y,t)dy, \quad \tilde{\mu_3}(t) = \tilde{h}(t)\int_0^1 \tilde{v}(y,t)dy$$

or, after some calculus

$$p(t) = -\frac{\tilde{\mu_3}(t)}{\left(\int_0^1 v(y,t)dy\right)\left(\int_0^1 \tilde{v}(y,t)dy\right)}\int_0^1 W(y,t)dy + \frac{\Delta\mu_3(t)}{\int_0^1 v(y,t)dy}, \quad t \in [0,T]. \tag{12}$$

Note that condition 2. of Theorem 1 provides that v and $\tilde{v}$ are positive in $\overline{Q}$.

Following the proof of Theorem 2 of [6] we also obtain the expression for the derivative of p, namely

$$\begin{aligned} q(t) =& \frac{\Delta\mu_3'(t)}{\mu_2(t)} + \frac{a(\mu_1(t))W_y(0,t) - a(\mu_2(t))W_y(1,t)}{\mu_2(t)h(t)} \\ &+ \frac{p(t)}{\mu_2(t)}\left[\frac{\tilde{v}(1,t)a(\mu_2(t)) - \tilde{v}(0,t)a(\mu_1(t))}{h(t)\tilde{h}(t)} - \int_0^1 f(yh(t),t)dy \right. \\ &\left. - \tilde{h}(t)\int_0^1 dy\int_0^1 yf_z(yz,t)\Big|_{z=\tilde{h}(t)+\sigma(h(t)-\tilde{h}(t))} d\sigma\right]. \end{aligned} \tag{13}$$

We also have that

$$\begin{aligned} W(y,t) =& \int_0^t\int_0^1 G(y,t;\eta,\tau)\Big[\Big(-\frac{\eta\tilde{h}'(\tau)}{h(\tau)\tilde{h}(\tau)}\tilde{v}_\eta(\eta,\tau) - \frac{h(\tau)+\tilde{h}(\tau)}{h^2(\tau)\tilde{h}^2(\tau)}a(\tilde{v}(\eta,\tau)) \\ &+ \int_0^1 \eta f_z(\eta z,\tau)\Big|_{z=\tilde{h}(\tau)+\sigma(h(\tau)-\tilde{h}(\tau))} d\sigma\Big)p(\tau) + \frac{q(\tau)}{h(\tau)} \\ &+ W(\eta,\tau)\int_0^1 a'(z)\Big|_{z=\tilde{v}(\eta,\tau)+\sigma(v(\eta,\tau)-\tilde{v}(\eta,\tau))} d\sigma\Big] d\eta d\tau, \quad (y,t) \in \overline{Q}, \end{aligned} \tag{14}$$

where $G(y,t;\eta,\tau)$ is the Green function for the linear partial differential equation

$$W_t = \left(\frac{a(v(y,t))}{h^2(t)}W_y\right)_y + \frac{yh'(t)}{h(t)}W_y \tag{15}$$

subject to the homogenous initial and boundary conditions

$$W(y,0) = 0, \qquad y \in [0,1] \tag{16}$$

$$W(0,t) = W(1,t) = 0, \qquad t \in [0,T]. \tag{17}$$

The expression for the derivative $W_y(y,t)$ is obtained by replacing $G(y,t;\eta,\tau)$ with $G_y(y,t;\eta,\tau)$ in (14). In [6], the uniqueness of the solution of the problem (1)–(4) is obtained by remarking that when $\mu_3 = \tilde{\mu}_3$, i.e. $\Delta\mu_3 = 0$, then the system of equations (12)–(14) is a homogenous system of Volterra integral equations of second kind with integrable kernels for the triplet solution $(p(t), q(t), W(y,t))$.

For the stability, one can observe that the inhomogenous free terms in equations (12) and (13) are

$$\frac{\Delta\mu_3(t)}{\int_0^1 v(y,t)dy} \quad \text{and} \quad \frac{\Delta\mu_3'(t)}{\mu_2(t)},$$

respectively. These terms are bounded by $\frac{1}{M_0}||\Delta\mu_3||_{C^1[0,T]}$. Then the stability estimate (10) follows immediately.

Remark 1. From Theorem 3 we have the continuous dependence of h upon the input data μ_3 in the $C^1[0,T]$ norm. However, in practice the energy data μ_3, as given by (4), comes from measurement which is inherently contaminated with noise, see later on equations (30)–(32). Therefore, the input data μ_3 is in $C[0,T]$, but not in $C^1[0,T]$, and consequently, the derivative μ_3' of the noisy function μ_3 will be unstable. However, there exist numerous numerical methods, see e.g. [9], which can stabilise the ill-posed process of numerical differentiation.

3 Solution of Direct Problem

There is no major difficulty in formally applying finite-difference methods to non-linear parabolic equations. The major difficulties are associated with the difference equations themselves. These are usually solved iteratively after being linearized in some way, as we will discuss later on.

In this section, we consider the direct initial-boundary value problem (6)–(8), where $h(t)$, $f(x,t)$, $a(u)$ and $\mu_i(t)$, $i \in \{1,2\}$ are known and the solution $u(x,t)$ is to be determined together with $\mu_3(t)$ defined by equation (4). To do so, we use the three-time levels finite difference scheme suggested by Lees [7].

The discrete form of our problem is as follows. We uniformly divide the fixed domain $Q = (0,1)\times(0,T)$ into M and N subintervals of equal step length Δy and Δt, where $\Delta y = 1/M$ and $\Delta t = T/N$, respectively. So, the solution at the node (i,j) is $v_{i,j} := v(y_i, t_j)$, where $y_i = i\Delta y$, $t_j = j\Delta t$, $h(t_j) = h_j$, $\phi(x_i) = \phi_i$, and $f(y_i,t_j) = f_{i,j}$ for $i = \overline{0,M}$, $j = \overline{0,N}$.

We develop the procedure described in [7] in order to solve the direct problem for the nonlinear parabolic equation (6), subject to the initial condition (7) and the Dirichlet boundary conditions (8). We need to define the standard difference operators D_+, D_-, and D_0, as follows:

$$D_+v(x_i,t_j) = \frac{v(x_{i+1},t_j) - v(x_i,t_j)}{\Delta y}, \quad D_-v(x_i,t_j) = \frac{v(x_i,t_j) - v(x_{i-1},t_j)}{\Delta y},$$
$$D_0v(x_i,t_j) = \frac{v(x_{i+1},t_j) - v(x_{i-1},t_j)}{2\Delta y}.$$

Finally, for any suitably defined function $k(x,t)$, we put

$$\bar{a}(k(x_i,t)) = a\left(\frac{k(x_i,t) + k(x_{i-1},t)}{2}\right).$$

For each $j = \overline{0,N}$ we put $v_{0,j} = \mu_1(j\Delta t)$ and $v_{M,j} = \mu_2(j\Delta t)$. Then the three time level scheme is given by

$$v_{i,0} = \phi_i, \qquad i = \overline{0,M}, \tag{18}$$

where we have that $\phi_0 = \mu_1(0)$ and $\phi_M = \mu_2(0)$,

$$v_{i,1} = v_{i,0} + \frac{\Delta t}{h_0^2} D_+ \left(\bar{a}(\phi_i) D_- \phi\right) + \frac{(\Delta t) y_i h_0'}{h_0} D_- \phi + (\Delta t) f_{i,0}, \qquad i = \overline{1, M-1}, \tag{19}$$

where $h_0' = h'(0)$ is given by (5),

$$\begin{aligned} v_{i,j+1} = v_{i,j-1} + \frac{2\Delta t}{h_j^2} D_+ \left(\bar{a}(v_{i,j}) D_- \hat{v}_{i,j}\right) + \frac{2(\Delta t) y_i h_j'}{h_j} D_- \hat{v}_{i,j} \\ + 2(\Delta t) f_{i,j}, \qquad i = \overline{1, M-1}, \quad j = \overline{1, N-1}, \end{aligned} \tag{20}$$

where $h_j' = h'(t_j)$, and

$$\hat{v}_{i,j} = \frac{v_{i,j+1} + v_{i,j} + v_{i,j-1}}{3}. \tag{21}$$

It is clear that the three-level difference scheme determines $v_{i,j+1}$ uniquely as the solution of a linear, well-conditioned, tridiagonal system of equations which can be solved using traditional linear algebra methods to advance the solution to the next time step. The equations (18) and (19) provide the necessary starting values for (20). In [7], the author proved that the above scheme is stable, second-order accurate and convergent for sufficiently small values of Δy and Δt. Although, equation (1) or (6) is nonlinear, the linearity is achieved in $v_{i,j+1}$ by evaluating all coefficients at a time level of known solution values in previous steps. The stability is preserved by averaging $v_{i,j}$ over three time levels as (21) and the accuracy is maintained by using central-difference approximations, [10].

Equation (20) can be put in a simpler form as

$$v_{i,j+1} = \hat{v}_{i,j-1} + A_{i,j} \hat{v}_{i-1,j} - B_{i,j} \hat{v}_{i,j} + C_{i,j} \hat{v}_{i+1,j} + 2(\Delta t) f_{i,j}, \tag{22}$$

where,

$$\begin{aligned} A_{i,j} &= \frac{2(\Delta t) a2_{i,j}}{h_j^2 (\Delta y)^2} - \frac{(\Delta t) y_i h_j'}{h_j \Delta y}, \quad B_{i,j} = \frac{2(\Delta t) a3_{i,j}}{h_j^2 \Delta y}, \quad C_{i,j} = \frac{2(\Delta t) a1_{i,j}}{h_j^2 (\Delta y)^2} + \frac{(\Delta t) y_i h_j'}{h_j \Delta y}, \\ a1_{i,j} &= \bar{a}(v(x_{i+1}, t_j)), \quad a2_{i,j} = \bar{a}(v(x_i, t_j)), \quad a3_{i,j} = a1_{i,j} + a2_{i,j}. \end{aligned}$$

As mentioned before, to ensure the stability we average the solution over three levels as

$$\begin{aligned} \hat{v}_{i-1,j-1} &= \frac{1}{3} \left(v_{i-1,j+1} + v_{i-1,j} + v_{i-1,j-1}\right), \\ \hat{v}_{i,j} &= \frac{1}{3} \left(v_{i,j+1} + v_{i,j} + v_{i,j-1}\right), \\ \hat{v}_{i+1,j-1} &= \frac{1}{3} \left(v_{i+1,j+1} + v_{i+1,j} + v_{i+1,j-1}\right). \end{aligned}$$

Then the final version of (22) becomes

$$\begin{aligned} -A_{i,j}^* v_{i-1,j+1} + (1 + B_{i,j}^*) v_{i,j+1} - C_{i,j}^* v_{i+1,j+1} = A_{i,j}^* v_{i-1,j} - B_{i,j}^* v_{i,j} + C_{i,j}^* v_{i+1,j} \\ + A_{i,j}^* v_{i-1,j-1} + (1 - B_{i,j}^*) v_{i,j-1} + C_{i,j}^* v_{i+1,j-1} \\ + 2(\Delta t) f_{i,j}, \ j = \overline{1, N}, \ i = \overline{2, (M-1)}, \end{aligned} \tag{23}$$

where $A^* = \frac{A}{3}$, $B^* = \frac{B}{3}$ and $C^* = \frac{C}{3}$. At each time step t_j for $j = \overline{1,(N-1)}$, using the Dirichlet boundary conditions (8), the above difference equation can be reformulated as a $(M-1)\times(M-1)$ system of linear equations of the form,

$$L\mathbf{u} = \mathbf{b}, \tag{24}$$

where

$$\mathbf{u} = (v_{2,j+1}, v_{3,j+1}, ..., v_{M-1,j+1})^{tr}, \quad \mathbf{b} = (b_2, b_3, ..., b_{M-1})^{tr}.$$

and

$$L = \begin{pmatrix} 1+B^*_{1,j} & -C^*_{1,j} & 0 & \cdots & 0 & 0 & 0 \\ -A^*_{2,j} & 1+B^*_{2,j} & -C^*_{2,j} & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & -A^*_{M-2,j} & 1+B^*_{M-2,j} & -C^*_{M-2,j} \\ 0 & 0 & 0 & \cdots & 0 & -A^*_{M-1,j} & 1+B^*_{M-1,j} \end{pmatrix},$$

$$\begin{aligned} b_2 &= A^*_{1,j}v_{0,j} - B^*_{1,j}v_{1,j} + C^*_{1,j}v_{2,j} + A^*_{1,j}v_{0,j-1} + (1-B^*_{1,j})v_{1,j-1} + C^*_{1,j}v_{2,j-1} \\ &\quad + 2(\Delta t)f_{1,j} + A^*_{1,j}v_{0,j+1}, \\ b_i &= A^*_{i-1,j}v_{i,j} - B^*_{i,j}v_{i,j} + C^*_{i,j}v_{i+1,j} + A^*_{i,j}v_{i-1,j-1} + (1-B^*_{i,j})v_{i,j-1} \\ &\quad + C^*_{i,j}v_{i+1,j-1} + 2(\Delta t)f_{i,j}, \qquad\qquad i = \overline{3,(M-2)}, \\ b_{M-1} &= A^*_{M-1,j}v_{M-2,j} - B^*_{M-1,j}v_{M-1,j} + C^*_{M-1,j}v_{M,j} + A^*_{M-1,j}v_{M-2,j-1} + (1-B^*_{M-1,j})v_{M-1,j-1} \\ &\quad + C^*_{M-1,j}v_{M+1,j-1} + 2(\Delta t)f_{M-1,j} + C^*_{M-1,j}v_{M,j+1}. \end{aligned}$$

3.1 Example

As an example, consider the problem (6)–(8) with $T = \ell = 1$ and

$$\begin{aligned} &a(v) = e^{-v}, \quad h(t) = 1+t, \quad h_0 = h(0) = 1, \quad \phi(h_0 y) = 1 + (1+y)^2, \\ &\mu_1(t) = 1 + e^t, \quad \mu_2(t) = (2+t)^2 + e^t, \quad f(h(t)y,t) = e^t + e^{-(1+y+yt)^2 - e^t}(4(1+y+yt)^2 - 2). \end{aligned}$$

The exact solution of the direct problem (6)–(8) is given by

$$v(y,t) = (1+y+yt)^2 + e^t$$

and the desired output (4) is

$$\mu_3(t) = \frac{(2+t)^3 - 1}{3} + (1+t)e^t.$$

The numerical and the exact solution for the interior solution are shown in Figure 1 and one can notice that a very good agreement is obtained because the direct problem is well-posed. Figure 2 shows the numerical solution in comparison with exact one for μ_3. The trapezoidal rule is employed to compute the integral in (4) based on the formula

$$\int_0^1 v(y,t_j)dy = \frac{1}{2M}\left(\mu_1(t_j) + \mu_2(t_j) + 2\sum_{i=1}^{M-1} v(y_i,t_j)\right), \qquad j = \overline{0,N}. \tag{25}$$

From this figure it can be seen that the numerical solution is in excellent agreement with the exact one.

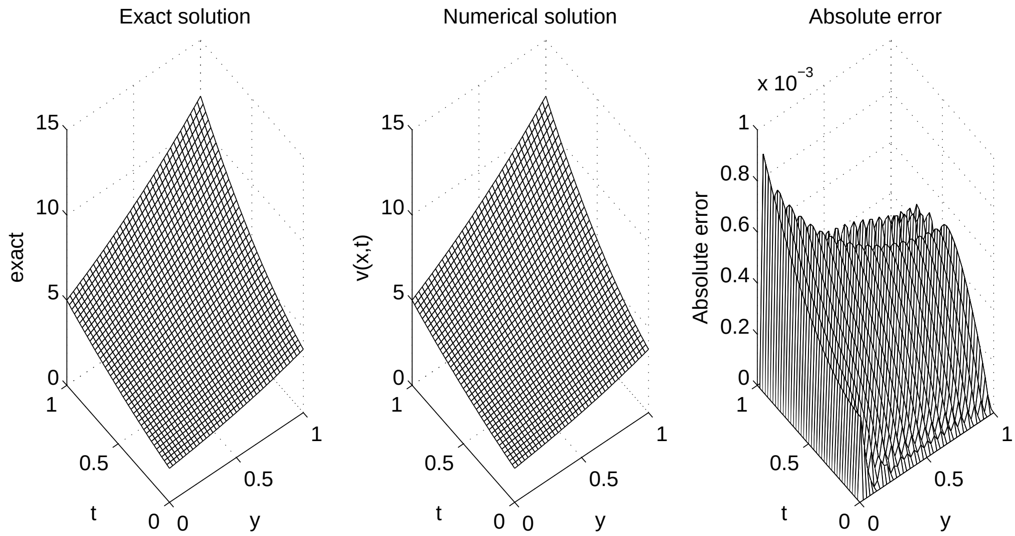

Figure 1: Exact and numerical solutions for $v(y,t)$ and the absolute error for the direct problem obtained with $M = N = 40$.

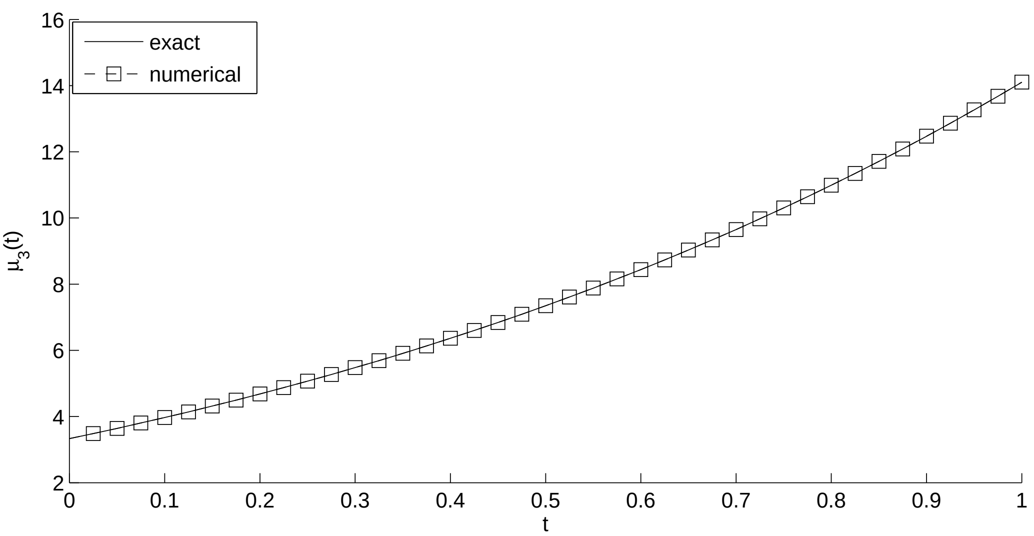

Figure 2: Exact and numerical integration for $\mu_3(t)$ for the direct problem obtained with $M = N = 40$.

4 Numerical Approach to the Inverse Problem

In the inverse problem, we assume that the free boundary $h(t)$ is unknown. The nonlinear inverse problem (6)–(9) can be reformulated as a nonlinear least-squares minimization of

$$F(h) = \left\| h(t) \int_0^1 v(y,t)dy - \mu_3(t) \right\|^2_{L^2[0,T]}, \tag{26}$$

defined over the set of admissible functions

$$h \in \Lambda_{ad} := \{ h \in C^1[0,T] \big| h(0) = h_0,\ h(t) > 0 \text{ for } t \in [0,T] \}. \tag{27}$$

The discretization of (26) is

$$F(\underline{h}) = \sum_{j=1}^{N} \left[h_j \int_0^1 v(y,t_j)dy - \mu_3(t_j) \right]^2, \tag{28}$$

where $\underline{h} = (h_j)_{j=\overline{1,N}}$. As it will be seen from the numerical results presented and discussed in the next section, it seems that there is no need to regularize the least-squares functional (26) by adding to it a Tikhonov penalty term of some norm of h, the problem being rather stable with respect to noise added in the input data $\mu_3(t)$.

The minimization of F subject to the physical constraints $\underline{h} > \underline{0}$ is accomplished using the MATLAB toolbox routine *lsqnonlin*, which does not require supplying by the user the gradient of the objective function (28), [8]. This routine attempts to find a minimum of a scalar function of several variables, starting from an initial guess, subject to constraints and this generally is referred to as a constrained nonlinear optimization.

We take bounds for the positive $h(t)$ say, we seek the components of the vector $\underline{h}$ in the interval $(10^{-10}, 10^3)$. We also take the parameters of the routine as follows:

- Number of variables $M = N = 40$.
- Maximum number of iterations $= 10^2 \times$ (number of variables).
- Maximum number of objective function evaluations $= 10^3 \times$ (number of variables).
- x Tolerance (xTol) $= 10^{-10}$.
- Function Tolerance (FunTol) $= 10^{-10}$.
- Nonlinear constraint tolerance $= 10^{-6}$.

In addition, when we solve the inverse problem we approximate

$$h'(t_j) = \frac{h(t_j) - h(t_{j-1})}{\Delta t} = \frac{h_j - h_{j-1}}{\Delta t}, \quad j = \overline{1,N}, \tag{29}$$

and we express $h'_0 := h'(0)$ as in (5). If there is noise in the measured data (4), we replace $\mu_3(t_j)$ in (28) by $\mu_3^\epsilon(t_j)$ given by

$$\mu_3^\epsilon(t_j) = \mu_3(t_j) + \epsilon_j, \quad j = \overline{1,N}, \tag{30}$$

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

$$\sigma = p \times \max_{t\in[0,T]} |\mu_3(t)|, \tag{31}$$

where p represents the percentage of noise. We use the MATLAB function *normrnd* to generate the random variables $\underline{\epsilon} = (\epsilon_j)_{j=\overline{1,N}}$ as follows:

$$\underline{\epsilon} = normrnd(0, \sigma, N). \tag{32}$$

5 Numerical Results and Discussion

In this section, we will describe the numerical results for our nonlinear inverse problem for two different example according to the linear and nonlinear (rational) variation of free boundary. Moreover, we add noise to the measured input data (9) to mimic the reality situation by using (30) via (32). To compute this coefficient we use the *lsqnonlin* routine combined with Trust-Region-reflective algorithm [8] to find the minimizer of the nonlinear functional (28). We also calculate the root mean square error ($rmse$) to analyse the error between the exact and numerically obtained coefficient, defined as,

$$rmse(h(t)) = \sqrt{\frac{1}{N}\sum_{j=1}^{N}\left(h_{numerical}(t_j) - h_{exact}(t_j)\right)^2}. \tag{33}$$

For simplicity, we take $T = 1$ and the initial guess $\underline{h}^{(0)} = \underline{1}$ for all examples.

Example 1

Consider the problem (1)–(4) with unknown coefficient $h(t)$, and solve this inverse problem with the following input data:

$$\begin{aligned}
\phi(x) &= (1+x)^2 + 1, \quad \mu_1(t) = 1 + e^t, \quad \mu_2(t) = (2+t)^2 + e^t,\\
\mu_3(t) &= \frac{(2+t)^3}{3} + (1+t)e^t - \frac{1}{3}, \quad a(u) = e^{-u},\\
f(x,t) &= e^t + e^{-(1+x)^2 - e^t}(4x^2 + 8x + 2), \quad h_0 = 1,
\end{aligned}$$

One can remark that the conditions of Theorems 1 and 2 are satisfied hence, the existence and uniqueness of solution hold. With this data the analytical solution of inverse problem (1)–(4) is given by

$$h(t) = 1 + t, \quad u(x,t) = (1+x)^2 + e^t. \tag{34}$$

Then

$$h(t) = 1 + t, \quad v(y,t) = u(yh(t), t) = (1 + y + yt)^2 + e^t, \tag{35}$$

is the analytical solution of the problem (6)–(9).

We consider the case where there is no noise, i.e. $p = 0$, and when there is $p = 2\%$ noise in the input data (9).

The functional (28), as a function of the number of iterations, is represented in Figure 3. From this figure it can be seen that the convergence is very fast in five and seven iterations for $p = 0$ and $p = 2\%$, respectively. The objective function (28) decreases rapidly and takes a stationary value of $O(10^{-7})$ and 0.3411, for $p = 0$ and $p = 2\%$, respectively. The numerical results for the corresponding unknown free boundary $h(t)$ are presented in Figure 4. From this figure it can be seen that the retrieved free boundary $h(t)$ is in very good agreement with the exact one in the case where no noise in the input data. While, when the input data is contaminated by $p = 2\%$ noise then we can see that the retrieved solution is stable and within the same range of errors as the input data is.

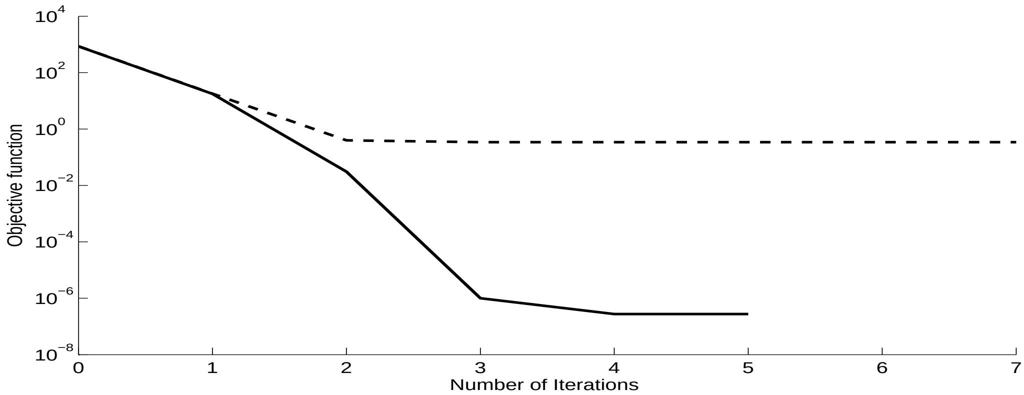

Figure 3: Objective function (28) without noise (—), and for $p = 2\%$ noise (- - -) for Example 1.

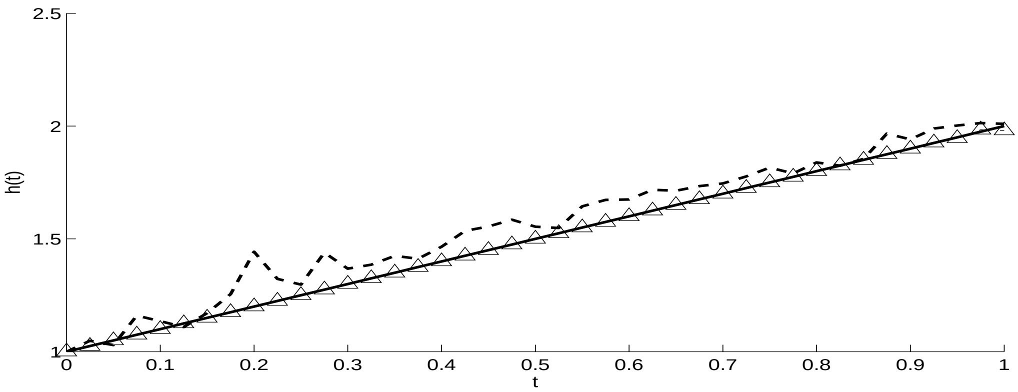

Figure 4: Free boundary $h(t)$, without noise (-$\triangle$-), and for $p = 2\%$ noise (- - -) in comparison with the exact solution (—), for Example 1.

The restored temperatures $v(y,t)$ and $u(x,t)$ for $p = 2\%$ noise are shown in Figures 5 and 6, respectively. From these figures it can be seen that the solutions are stable by being free of high oscillations and unbounded behaviour.

Overall form the numerical results presented for this example it can be seen that the inverse problem seems to be well-posed and that the numerical solutions are accurate and stable with respect to noise in the input data for both the free boundary $h(t)$ and the temperature/concentration $v(y,t)$ or $u(x,t)$.

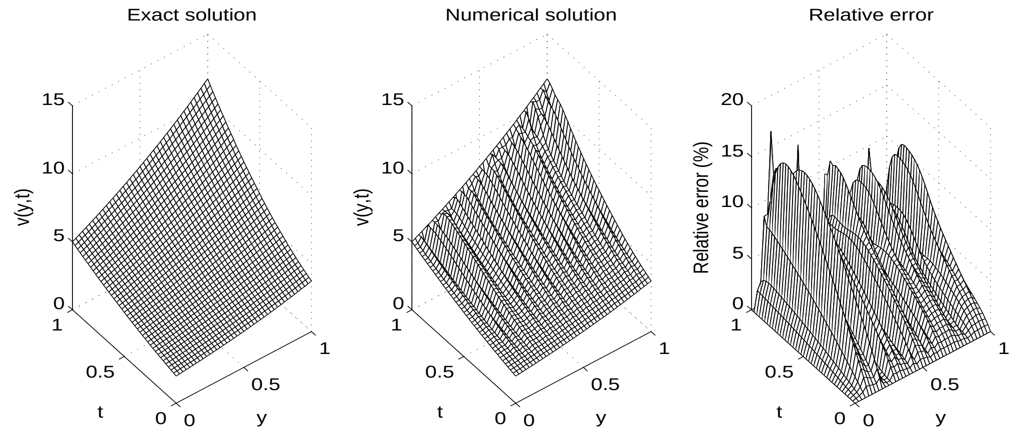

Figure 5: The analytical and numerical solutions, and the relative error for $v(y,t)$ for $p = 2\%$ noise for Example 1.

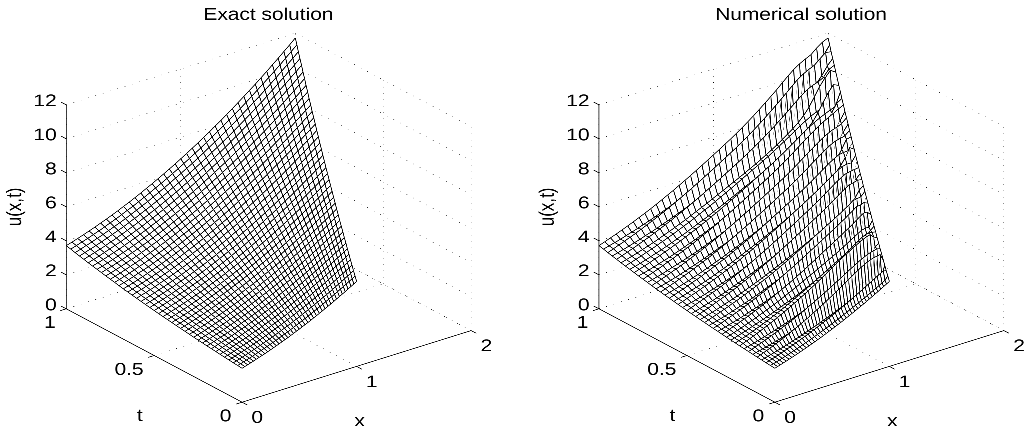

Figure 6: The analytical and numerical solutions for $u(x,t)$ for $p = 2\%$ noise for Example 1.

Example 2

In this example, we consider a more severe test case where the unknown function $h(t)$ is nonlinear with the following data

$$
\begin{aligned}
&\phi(x) = (1+x)^2 + 1, \quad \mu_1(t) = 1 + e^t, \quad \mu_2(t) = \left(\frac{2+t}{1+t}\right)^2 + e^t, \\
&\mu_3(t) = \frac{1}{3}\left(\frac{2+t}{1+t}\right)^3 + \frac{e^t}{1+t} - \frac{1}{3}, \quad a(u) = e^{-u}, \\
&f(x,t) = e^t + e^{-(1+x)^2 - e^t}\left(4x^2 + 8x + 2\right), \quad h_0 = 1.
\end{aligned}
$$

One can notice that the conditions of Theorems 1 and 2 are satisfied hence, the existence and uniqueness of solution holds. With this data, the analytical solution of the inverse problem (1)–(4) is given by

$$h(t) = \frac{1}{1+t}, \quad u(x,t) = (1+x)^2 + e^t. \tag{36}$$

Then

$$h(t) = \frac{1}{1+t}, \quad v(y,t) = u(yh(t),t) = \left(1 + \frac{y}{1+t}\right)^2 + e^t, \tag{37}$$

is the analytical solution of the problem (6)–(9).

We study the case of exact and noisy input data (9). The objective function (28), as a function of the number of iterations is presented in Figure 7. From this figure it can be seen that the functional decreases very fast to stationary value at $O(10^{-7})$ and 0.0188 in about 7 and 12 iterations, for $p = 0$ and $p = 2\%$ noise, respectively.

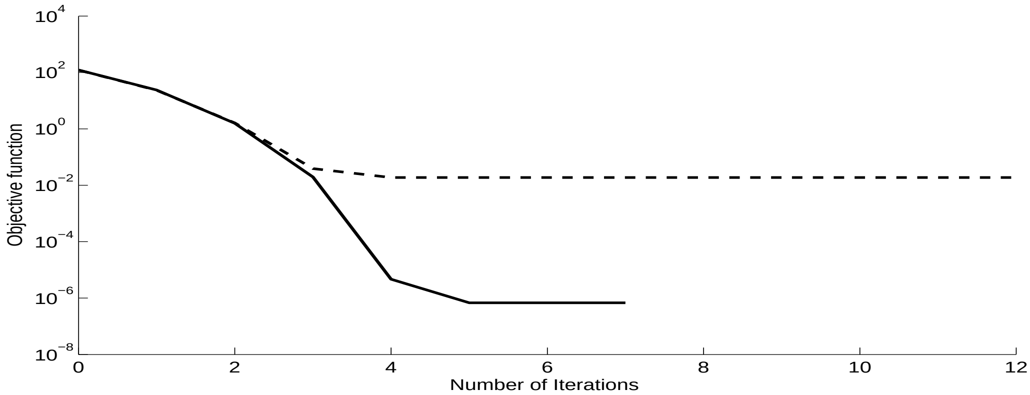

Figure 7: Objective function (28) without noise (—), and for $p = 2\%$ noise (- - -) for Example 2.

The numerical results for the corresponding free boundary $h(t)$ are presented in Figure 8. From this figure it can be seen that the identified free boundary is in very good agreement with the exact one in the absence of noise and this situation changes only a little when we perturb the input data by $p = 2\%$ noise.

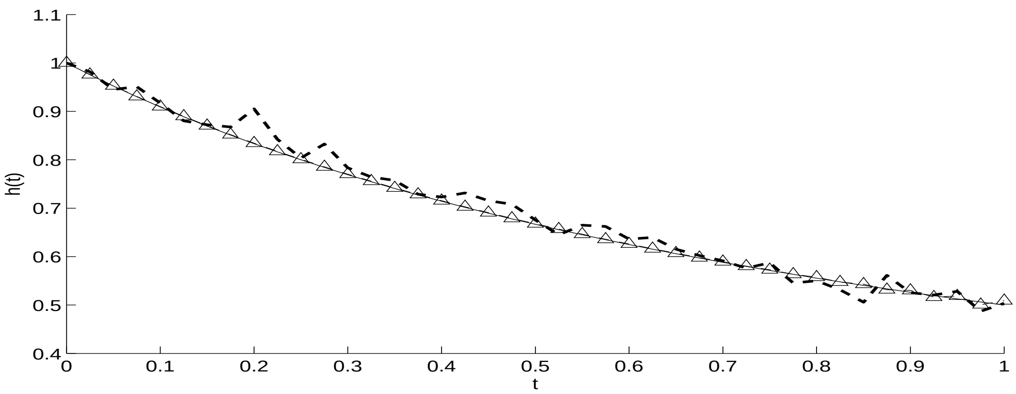

Figure 8: Free boundary $h(t)$, without noise (-△-), and with $p = 2\%$ noise (- - -) in comparison with the exact solution (—), for Example 2.

The numerical solutions for $v(y,t)$ and $u(x,t)$ are shown in Figure 9 and 10, respectively, in comparison with the exact solutions for $p = 2\%$ noise. As in Example 1, stable numerical solutions are obtained.

One can conclude that the inverse problem is well-posed since small errors in the measurement in (4) cause only small errors in the retrieved pair solution $(h(t),\ u(x,t))$. Consequently, we can say that the problem depends continuously on the input data.

Finally, for completeness, other details about the number of iterations, number of function evaluations, objective function value at final iteration and $rmse(h)$ for Examples 1 and 2 are given in Table 1. For this table it can be seen that accurate and stable numerical solutions are rapidly achieved by the iterative MATLAB toolbox routine *lsqnonlin*.

Table 1: Number of iterations, number of function evaluations, value of the objective function (28) at final iteration and *rmse* values (33), for Examples 1 and 2.

		$p = 0$	$p = 2\%$
Example 1	No. of iterations	5	7
	No. of function evaluations	252	336
	Function value at final iteration	$2E-7$	0.3411
	$rmse(h)$	0.0035	0.0793
Example 2	No. of iterations	7	12
	No. of function evaluations	336	546
	Function value at final iteration	$6E-7$	0.0188
	$rmse(h)$	0.0023	0.0212

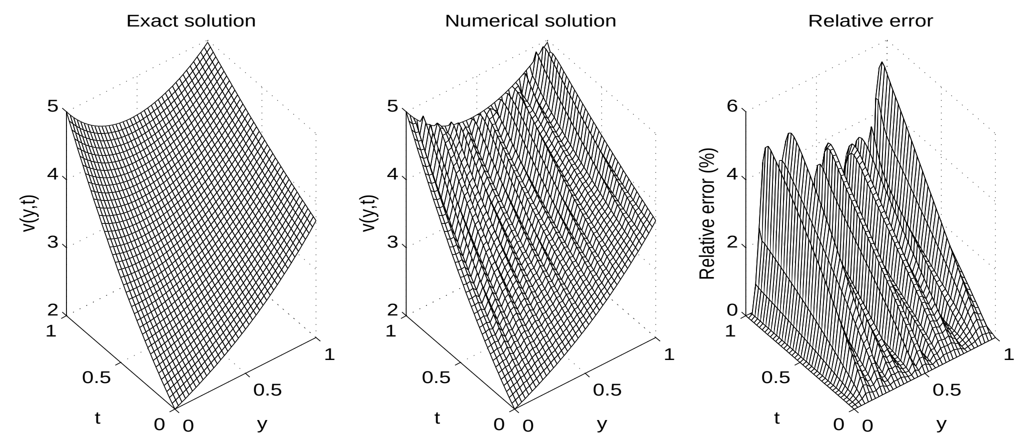

Figure 9: The analytical and numerical solutions and the relative error for $v(y,t)$ for $p = 2\%$ noise for Example 2.

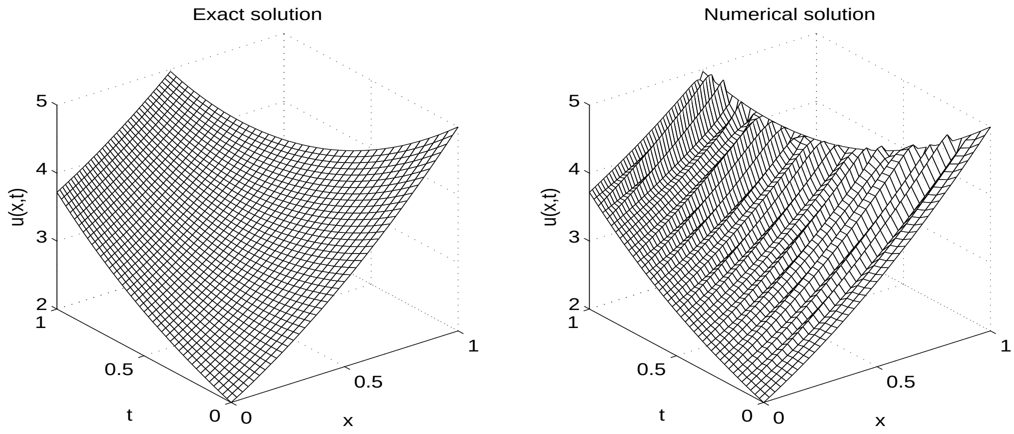

Figure 10: The analytical and numerical solutions for $u(x,t)$ for $p = 2\%$ noise for Example 2.

6 Conclusions

The inverse problem concerning the identification of free boundary $h(t)$ and the temperature $u(x,t)$ in the heat equation with nonlinear diffusivity $a(u)$ has been investigated. The additional condition which ensures a unique solution is given by the energy/mass specification $\mu_3(t)$ given by equation (4). As with other free surface problems, it turns out that the problem is well-posed if the data μ_3 is smooth. The direct solver based on a three-level finite difference scheme is developed. The inverse solver is based on a nonlinear least-squares minimization which is solved using the MATLAB toolbox routine *lsqnonlin*. As expected, for exact data, the numerical results obtained are very accurate. For noisy data μ_3^ϵ which consist of a random perturbation of the exact data μ_3, the results for $h(t)$, $v(y,t)$ and $u(x,t)$ are still stable and accurate. The instability is only manifested in the derivative $h'(t)$ for which the use of a regularization method would be warranted.

Acknowledgments

M.S. Hussein would like to thank the Higher Committee of Education Development in Iraq (HCEDiraq) for their financial support in this research.

References

[1] Broadbridge, P., Tritscher, P. and Avagliano, A. (1993) Free boundary problems with nonlinear diffusion, *Mathematical and Computer Modelling*, **18**, 15–34.

[2] Cannon, J.R. and Duchateau, P. (1973) Determining unknown coefficients in a nonlinear heat conduction problem, *SIAM Journal on Applied Mathematics*, **24**, 298–314.

[3] Cannon, J.R. and Duchateau, P. (1980) An inverse problem for a nonlinear diffusion equation, *SIAM Journal on Applied Mathematics*, **39**, 272–289.

[4] Cannon, J.R. and Hoek, J. (1986) Diffusion subject to the specification of mass, *Journal of Mathematical Analysis and Applications*, **115**, 517–529.

[5] Friedman, A. (1964) *Partial Differential Equations of Parabolic Type*, Prentice-Hall, Englewood Cliffs, NJ.

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

[7] Lees, M. (1966) A linear three-level difference scheme for quasilinear parabolic equations, *Mathematics of Computation*, **20**, 516–522.

[8] Mathworks R2012 Documentation Optimization Toolbox-Least Squares (Model Fitting) Algorithms, available from www.mathworks.com/help/toolbox/optim/ug /brnoybu.html.

[9] Murio, D.A.(1993) *The Mollification Method and the Numerical Solution of Ill-posed Probelms*, Wiley, New York.

[10] Smith, G.D. (1985) *Numerical Solution of Partial Differential Equations: Finite Difference Methods*, Oxford Applied Mathematics and Computing Science Series, Third Edition.

[11] Wang, P. and Zheng, K. (2002) Determination of an unknown coefficient in a nonlinear heat equation, *Journal of Mathematical Analysis and Applications*, **271**, 525–533.