East Asian Journal on Applied Mathematics
doi: 10.4208/eajam.100913.061113a

Vol. **3**, No. 4, pp. 295-310
November 2013

Free Boundary Determination in Nonlinear Diffusion

M. S. Hussein[1,2,*], D. Lesnic[1] and M. Ivanchov[3]

[1] *Department of Applied Mathematics, University of Leeds, Leeds LS2 9JT, United Kingdom.*
[2] *Department of Mathematics, College of Science, University of Baghdad, Baghdad, Iraq.*
[3] *Faculty of Mechanics and Mathematics, Department of Differential Equations, Ivan Franko National University of Lviv, 1, Universytetska str., Lviv, 79000, Ukraine.*

Received 10 September 2013; Accepted (in revised version) 6 November 2013.

Available online 28 November 2013

Abstract. Free boundary problems with nonlinear diffusion occur in various applications, such as solidification over a mould with dissimilar nonlinear thermal properties and saturated or unsaturated absorption in the soil beneath a pond. In this article, we consider a novel inverse problem where a free boundary is determined from the mass/energy specification in a well-posed one-dimensional nonlinear diffusion problem, and a stability estimate is established. The problem is recast as a nonlinear least-squares minimisation problem, which is solved numerically using the *lsqnonlin* routine from the MATLAB toolbox. Accurate and stable numerical solutions are achieved. For noisy data, instability is manifest in the derivative of the moving free surface, but not in the free surface itself nor in the concentration or temperature.

AMS subject classifications: 35R35, 35K55, 49N45, 65M06

Key words: Nonlinear diffusion, free boundary problem, finite difference method.

1. Introduction

Many industrial and scientific applications involving inverse problems have ensured that this mathematical field has undergone extensive development over several decades, including a recent emphasis on nonlinear inverse problems — e.g. the Stefan solidification problem involving nonlinear diffusion with a free boundary [1], the determination of unknown coefficients together with the temperature in a nonlinear heat conduction problem [2,3], and the procedure to find an approximate stable solution to the unknown

*Corresponding author. *Email addresses:* `mmmsh@leeds.ac.uk` (M.S. Hussein), `amt5ld@maths.leeds.ac.uk` (D. Lesnic), `ivanchov@franko.lviv.ua` (M.I. Ivanchov)

coefficient from over-specified data based on the finite difference method combined with the Tikhonov regularisation approach [11].

In this article, we consider the problem of identifying the free boundary in a nonlinear diffusion problem. We formulate the inverse problem under investigation in Section 2. The respective numerical methods for solving the direct and inverse problems are described in Sections 3 and 4, and the numerical results are discussed in Section 5. Our final conclusions are presented in Section 6.

2. Mathematical Formulation

The nonlinear one-dimensional diffusion problem involves the partial differential equation

$$\frac{\partial u(x,t)}{\partial t} = \frac{\partial}{\partial x}\left(a(u)\frac{\partial u(x,t)}{\partial x}\right) + f(x,t)\,, \quad (x,t)\in\Omega \tag{2.1}$$

where the domain $\Omega = \{(x,t) : 0 < x < h(t), 0 < t < T < \infty\}$ has the unknown free smooth boundary $x = h(t) > 0$, subject to the initial condition

$$u(x,0) = \phi(x)\,, \quad 0 \le x \le h(0) =: h_0 \tag{2.2}$$

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

$$u(0,t) = \mu_1(t)\,, \quad u(h(t),t) = \mu_2(t)\,, \quad 0 \le t \le T\,. \tag{2.3}$$

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

$$\int_0^{h(t)} u(x,t)dx = \mu_3(t)\,, \quad 0 \le t \le T\,, \tag{2.4}$$

which represents the specification of mass/energy of the diffusion system [4]. The six functions $a(u) > 0$, $\phi(x)$, $\mu_i(t)$ for $i \in \{1,2,3\}$, and $f(x,t)$ are given. Physically, $u(x,t)$ represents the concentration or temperature, $a(u)$ the diffusivity, and $f(x,t)$ a source or sink. The function pair $(h(t) > 0, u(x,t)) \in C^1[0,T] \times C^{2,1}(\overline{\Omega})$ satisfying Eqs. (2.1)–(2.4) is the solution of the problem, under the following existence and uniqueness theorems [6].

Theorem 2.1. (Existence)

Assume that:

1. $\phi(x) \in C^2[0,h_0]$, $\mu_i(t) \in C^1[0,T]$ *for* $i \in \{1,2,3\}$, $f(x,t) \in C^{1,0}([0,H_1]\times[0,T])$, *and* $a(u) \in C^1[M_0,M_1]$;

2. $\phi(x) > 0$ *for* $x \in [0,h_0]$, $\mu_i(t) > 0$ *for* $t \in [0,T]$, $i \in \{1,2,3\}$, $f(x,t) \ge 0$ *for* $(x,t) \in [0,H_1]\times[0,T]$, *and* $a(u) \ge a_0 > 0$ *for* $u \in [M_0,M_1]$ *where* a_0 *is some given constant; and*

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 (2.1)–(2.4) *is locally solvable (in time).*

Theorem 2.2. (Uniqueness)
Suppose that not only condition 2 of Theorem 2.1 *but also the condition*

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

holds. Then a solution of the inverse problem (2.1)–(2.4) *is unique.*

The constants H_1, M_0 and M_1 in these theorems have the following meaning for the heat equation (2.1) — cf. the maximum principle [5]:

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

We can also obtain a formula for $h'(0)$ by differentiating Eq. (2.4) with time and using Eqs. (2.1)–(2.3):

$$h'(0)=\frac{\mu_3'(0)-a(\mu_2(0))\phi'(h_0)+a(\mu_1(0))\phi'(0)-\int_0^{h_0}f(x,0)dx}{\mu_2(0)}\,. \tag{2.5}$$

Under a change of variable $y=x/h(t)$, the inverse problem (2.1)–(2.4) reduces to the following equivalent problem for the unknowns $h(t)$ and $v(y,t):=u(yh(t),t)$ in a rectangular domain [6]:

$$\frac{\partial v(y,t)}{\partial t}=\frac{1}{h^2(t)}\frac{\partial}{\partial y}\left(a(v)\frac{\partial v(y,t)}{\partial y}\right)+\frac{yh'(t)}{h(t)}\frac{\partial v(y,t)}{\partial y}+f(yh(t),t)\,,\ (y,t)\in Q \tag{2.6}$$

where $Q=\{(y,t):0<y<1,0<t<T\}$, subject to the initial condition

$$v(y,0)=\phi(h_0y)\,,\quad 0\le y\le 1 \tag{2.7}$$

and the boundary and over-determination conditions

$$v(0,t)=\mu_1(t)\,,\quad v(1,t)=\mu_2(t)\,,\quad 0\le t\le T\,, \tag{2.8}$$
$$h(t)\int_0^1 v(y,t)dy=\mu_3(t)\,,\quad 0\le t\le T\,. \tag{2.9}$$

At the end of this section, we establish the continuous dependence of the free boundary $h(t)$ on the input energy data (2.4).

Theorem 2.3. (Stability)
Suppose that the conditions of Theorem 2.1 *are satisfied. Let μ_3 and $\tilde{\mu}_3$ be two data in* (2.4) *and let ($h(t)$, $u(x,t)$) and ($\tilde{h}(t)$, $\tilde{u}(x,t)$) be the corresponding solutions of the inverse problem* (2.1)–(2.4). *Then there is a positive constant C such that the following stability estimate holds:*

$$\|h-\tilde{h}\|_{C^1[0,T]}+\|v-\tilde{v}\|_{C^{1,0}(\overline{\Omega})}\le C\|\mu_3-\tilde{\mu_3}\|_{C^1[0,T]}\,, \tag{2.10}$$

where

$$v(y,t)=u(yh(t),t)\,,\quad \tilde{v}(y,t)=\tilde{u}(y\tilde{h}(t),t)\,,\quad (y,t)\in Q\,. \tag{2.11}$$

Proof. In order to establish the stability estimate (2.10), we follow the uniqueness proof given in Ref. [6]. If $p(t):=h(t)-\tilde{h}(t)$, $q(t):=h'(t)-\tilde{h}'(t)$, $W(y,t):=v(y,t)-\tilde{v}(y,t)$ and $\Delta\mu_3(t):=\mu_3(t)-\tilde{\mu_3}(t)$, from Eq. (2.9) one obtains

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

or after some calculus

$$p(t)=-\frac{\tilde{\mu_3}(t)}{\left(\int_0^1 v(y,t)dy\right)\left(\int_0^1\tilde{v}(y,t)dy\right)}\int_0^1 W(y,t)dy+\frac{\Delta\mu_3(t)}{\int_0^1 v(y,t)dy}\,,\qquad t\in[0,T]\,. \tag{2.12}$$

Note that condition 2 of Theorem 2.1 implies that v and $\tilde{v}$ are positive in $\overline{Q}$. Following the proof of Theorem 2.2 in Ref. [6], we obtain the expression for the derivative of p — viz.

$$\begin{aligned}q(t)=&\frac{\Delta\mu_3'(t)}{\mu_2(t)}+\frac{a(\mu_1(t))W_y(0,t)-a(\mu_2(t))W_y(1,t)}{\mu_2(t)h(t)}\\&+\frac{p(t)}{\mu_2(t)}\left[\frac{\tilde{v}(1,t)a(\mu_2(t))-\tilde{v}(0,t)a(\mu_1(t))}{h(t)\tilde{h}(t)}-\int_0^1 f(yh(t),t)dy\right.\\&\left.-\tilde{h}(t)\int_0^1 dy\int_0^1 yf_z(yz,t)\Big|_{z=\tilde{h}(t)+\sigma(h(t)-\tilde{h}(t))}d\sigma\right]\,.\end{aligned} \tag{2.13}$$

We also have that

$$\begin{aligned}W(y,t)=&\int_0^t\int_0^1 G(y,t;\eta,\tau)\left[\left(-\frac{\eta\tilde{h}'(\tau)}{h(\tau)\tilde{h}(\tau)}\tilde{v}_\eta(\eta,\tau)-\frac{h(\tau)+\tilde{h}(\tau)}{h^2(\tau)\tilde{h}^2(\tau)}a(\tilde{v}(\eta,\tau))\right.\right.\\&\left.+\int_0^1\eta f_z(\eta z,\tau)\Big|_{z=\tilde{h}(\tau)+\sigma(h(\tau)-\tilde{h}(\tau))}d\sigma\right)p(\tau)+\frac{q(\tau)}{h(\tau)}\\&\left.+W(\eta,\tau)\int_0^1 a'(z)\Big|_{z=\tilde{v}(\eta,\tau)+\sigma(v(\eta,\tau)-\tilde{v}(\eta,\tau))}d\sigma\right]d\eta d\tau\,,\quad (y,t)\in\overline{Q}\,,\end{aligned} \tag{2.14}$$

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

$$W_t = \left(\frac{a(v(y,t))}{h^2(t)}W_y\right)_y + \frac{yh'(t)}{h(t)}W_y \tag{2.15}$$

subject to the homogenous initial and boundary conditions

$$W(y,0) = 0\,, \quad y \in [0,1]\,, \tag{2.16}$$

$$W(0,t) = W(1,t) = 0\,, \quad t \in [0,T]\,. \tag{2.17}$$

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 Eq. (2.14). In Ref. [6], the uniqueness of the solution of the problem (2.1)–(2.4) is obtained by remarking that when $\mu_3 = \tilde{\mu}_3$ (i.e. $\Delta\mu_3 = 0$) then Eqs. (2.12)–(2.14) constitute an homogenous system of Volterra integral equations of the second kind with integrable kernels and the triplet solution $(p(t), q(t), W(y,t))$. For the stability, one can observe that the inhomogeneous free terms in Eqs. (2.12) and (2.13) 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 $M_0{}^{-1}||\Delta\mu_3||_{C^1[0,T]}$, and the stability estimate (2.10) follows immediately. □

Remark 2.1. From Theorem 2.3, there is 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 given by Eq. (2.4) comes from measurement, which is inherently contaminated with noise — cf. Eqs. (4.5)–(4.7) below. The input data μ_3 is therefore in $C[0,T]$ but not in $C^1[0,T]$, and consequently the derivative μ_3' of the noisy function μ_3 is unstable. However, there are many numerical methods that can stabilise the ill-posed process of numerical differentiation — e.g. see Ref. [9].

3. Solution of the Direct Problem

We now consider the direct initial-boundary value problem (2.6)–(2.8) 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 Eq. (2.4). There is no major difficulty in formally applying finite difference methods to nonlinear parabolic equations — the main difficulties are associated with the consequent difference equations, which are usually solved iteratively after being linearised in some way (see later). We use the three-time-level finite difference scheme suggested by Lees [7].

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. The solution at the node (i,j) is thus $v_{i,j} := v(y_i, t_j)$, 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 $i=\overline{0,M}$, $j=\overline{0,N}$. In order to solve the direct problem for the nonlinear parabolic equation (2.6) subject to the initial condition (2.7) and the Dirichlet boundary conditions (2.8), we define the standard difference operators

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

and 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 $v_{M,j}=\mu_2(j\Delta t)$, so the three-time-level scheme is

$$v_{i,0}=\phi_i\,,\ i=\overline{0,M}\quad\text{where } \phi_0=\mu_1(0)\ \text{ and }\ \phi_M=\mu_2(0)\,, \tag{3.1}$$
$$v_{i,1}=v_{i,0}+\frac{\Delta t}{h_0^2}D_+\left(\bar{a}(\phi_i)D_-\phi\right)+\frac{(\Delta t)y_ih_0'}{h_0}D_-\phi+(\Delta t)f_{i,0}\,,\quad i=\overline{1,M-1} \tag{3.2}$$

where $h_0'=h'(0)$ is given by Eq. (2.5),

$$v_{i,j+1}=v_{i,j-1}+\frac{2\Delta t}{h_j^2}D_+\left(\bar{a}(v_{i,j})D_-\hat{v}_{i,j}\right)+\frac{2(\Delta t)y_ih_j'}{h_j}D_-\hat{v}_{i,j}+2(\Delta t)f_{i,j} \tag{3.3}$$

where $h_j'=h'(t_j)$, for $i=\overline{1,M-1}$, $j=\overline{1,N-1}$ and

$$\hat{v}_{i,j}=\frac{v_{i,j+1}+v_{i,j}+v_{i,j-1}}{3}. \tag{3.4}$$

It is clear that the three-time-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. Eqs. (3.1) and (3.2) provide the necessary starting values for Eq. (3.3). For sufficiently small values of Δy and Δt, the scheme is stably second-order accurate and convergent [7]. Eq. (2.1) and Eq. (2.6) are nonlinear, but 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 in (3.4), and the accuracy is maintained by using central difference approximations [10].

Eq. (3.3) can be rendered in the simpler form

$$v_{i,j+1}=\hat{v}_{i,j-1}+A_{i,j}\hat{v}_{i-1,j}-B_{i,j}\hat{v}_{i,j}+C_{i,j}\hat{v}_{i+1,j}+2(\Delta t)f_{i,j}\,, \tag{3.5}$$

where

$$A_{i,j} = \frac{2(\Delta t)a2_{i,j}}{h_j^2(\Delta y)^2} - \frac{(\Delta t)y_i h_j'}{h_j \Delta y}\,, \quad B_{i,j} = \frac{2(\Delta t)a3_{i,j}}{h_j^2 \Delta y}\,, \quad C_{i,j} = \frac{2(\Delta t)a1_{i,j}}{h_j^2(\Delta y)^2} + \frac{(\Delta t)y_i h_j'}{h_j \Delta y}\,,$$

with $a1_{i,j} = \bar{a}(v(x_{i+1}, t_j))$, $a2_{i,j} = \bar{a}(v(x_i, t_j))$, $a3_{i,j} = a1_{i,j} + a2_{i,j}$. The solution is thus averaged over three levels as

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

and the resulting version of Eq. (3.5) is then

$$\begin{aligned}
&-A^*_{i,j}v_{i-1,j+1} + (1+B^*_{i,j})v_{i,j+1} - C^*_{i,j}v_{i+1,j+1}\\
&= A^*_{i,j}v_{i-1,j} - B^*_{i,j}v_{i,j} + C^*_{i,j}v_{i+1,j} + A^*_{i,j}v_{i-1,j-1} + (1 - B^*_{i,j})v_{i,j-1} + C^*_{i,j}v_{i+1,j-1} + 2(\Delta t)f_{i,j}\,,\\
&\qquad j = \overline{1,N}\,,\ i = \overline{2,(M-1)}\,,
\end{aligned} \tag{3.6}$$

where $A^* = A/3$, $B^* = B/3$ and $C^* = C/3$. At each time step t_j for $j = \overline{1,(N-1)}$, using the Dirichlet boundary conditions (2.8) this difference equation can be reformulated as an $(M-1) \times (M-1)$ system of linear equations of form

$$L\mathbf{u} = \mathbf{b}, \tag{3.7}$$

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

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

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

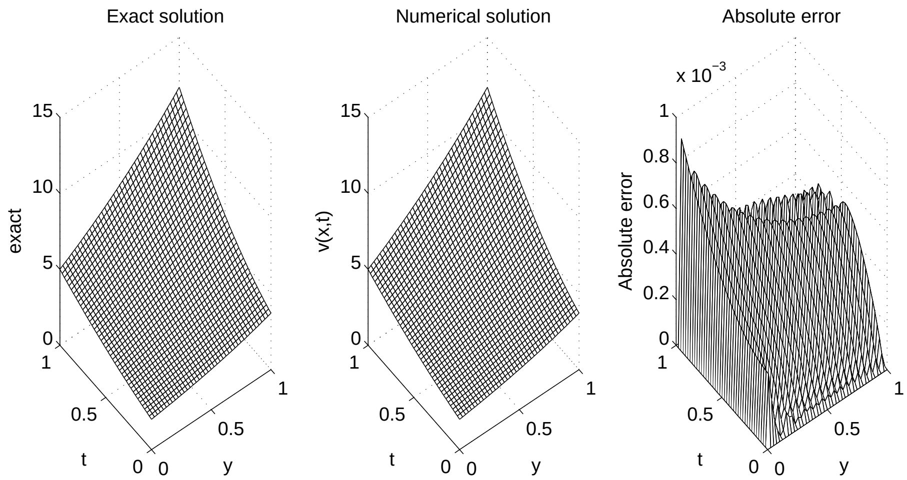

Figure 1: Exact and numerical solutions for $v(y,t)$, and the absolute error for the direct problem obtained with $M = N = 40$.

Example 3.1. Consider the problem (2.6)–(2.8) with $T = 1$ and

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

The exact solution of the direct problem (2.6)–(2.8) is given by

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

and the desired output (2.4) is

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

The numerical and exact solution for the interior solution shown in Fig. 1 are in very good agreement. The trapezoidal rule was employed to compute the integral in Eq. (2.4) — viz.

$$\int_0^1 v(y,t_j)dy = \frac{1}{2M}\left(\mu_1(t_j) + \mu_2(t_j) + 2\sum_{i=1}^{M-1} v(y_i,t_j)\right), \quad j = \overline{0,N}\,. \tag{3.8}$$

As shown in Fig. 2, the numerical solution and the exact solution for μ_3 are in excellent agreement.

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 (2.6)–(2.9) can be reformulated as a nonlinear least-squares min-

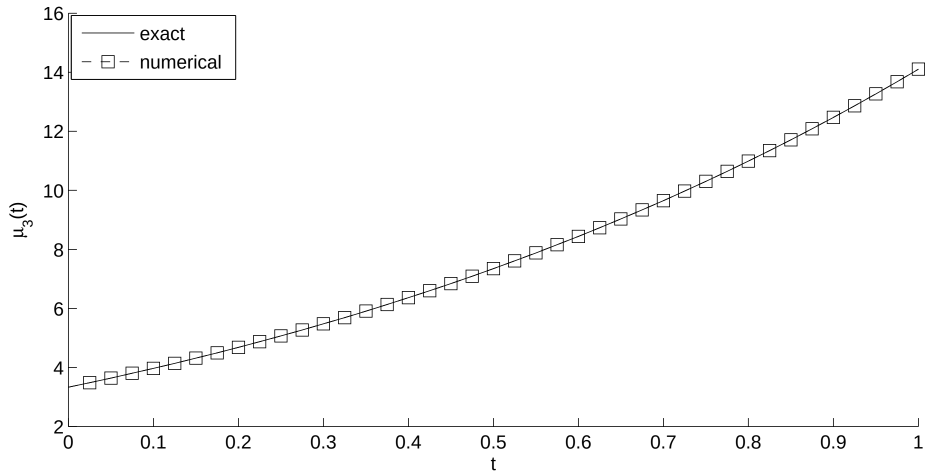

Figure 2: Exact and numerical integration for $\mu_3(t)$ for the direct problem obtained with $M = N = 40$.

imisation of

$$F(h) = \left\| h(t) \int_0^1 v(y,t)dy - \mu_3(t) \right\|^2_{L^2[0,T]}, \tag{4.1}$$

defined over the set of admissible functions

$$h \in \Lambda_{ad} := \{h \in C^1[0,T] \big| h(0) = h_0,\ h(t) > 0 \text{ for } t \in [0,T]\}. \tag{4.2}$$

The discretisation of Eq. (4.1) is

$$F(\underline{h}) = \sum_{j=1}^{N} \left[h_j \int_0^1 v(y,t_j)dy - \mu_3(t_j) \right]^2, \tag{4.3}$$

where $\underline{h} = \left(h_j\right)_{j=\overline{1,N}}$. From the numerical results discussed in the next section, it seems that there is no need to regularise the least-squares functional (4.1) by adding a Tikhonov penalty term of some norm of h, with the problem being rather stable to noise added in the input data $\mu_3(t)$.

The minimisation of F subject to the physical constraints $\underline{h} > \underline{0}$ was accomplished using the MATLAB toolbox routine *lsqnonlin*, which does not require the user to supply the gradient of the objective function (4.3), [8]. This routine attempts to find a minimum of a scalar function of several variables starting from an initial guess, subject to constraints — generally referred to as constrained nonlinear optimisation. We took bounds for the positive $h(t)$ by seeking the components of the vector $\underline{h}$ in the interval $(10^{-10}, 10^3)$. The adopted parameters of the routine were 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 solving the inverse problem we approximated

$$h'(t_j) = \frac{h(t_j) - h(t_{j-1})}{\Delta t} = \frac{h_j - h_{j-1}}{\Delta t}, \quad j = \overline{1, N}, \tag{4.4}$$

with $h'_0 := h'(0)$ as in Eq. (2.5). If there was noise in the measured data in Eq. (2.4), we replaced $\mu_3(t_j)$ in Eq. (4.3) by $\mu_3^\epsilon(t_j)$ given by

$$\mu_3^\epsilon(t_j) = \mu_3(t_j) + \epsilon_j, \quad j = \overline{1, N}, \tag{4.5}$$

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

$$\sigma = p \times \max_{t \in [0,T]} |\mu_3(t)|, \tag{4.6}$$

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

$$\underline{\epsilon} = normrnd(0, \sigma, N). \tag{4.7}$$

5. Numerical Results and Discussion

Numerical results for our nonlinear inverse problem (2.1)–(2.4) were obtained for two examples, with a linear and nonlinear (rational) variation of the free boundary, respectively. Moreover, we added noise to the measured input data in Eq. (2.9) to mimic the real situation, by using Eq. (4.5) and Eq. (4.7). To compute the free boundary, we used the *lsqnonlin* routine combined with the Trust-Region-Reflective algorithm [8] to find the minimiser of the nonlinear functional (4.3); and to analyse the error between the exact and numerically obtained results, we calculated the root mean square error

$$rmse(h(t)) = \sqrt{\frac{1}{N} \sum_{j=1}^{N} \left(h_{numerical}(t_j) - h_{exact}(t_j)\right)^2}. \tag{5.1}$$

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

Example 5.1. Consider the problem (2.1)–(2.4) with unknown free boundary $h(t)$, and solve this inverse problem with the following input data:

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

The conditions of Theorems 2.1 and 2.2 are satisfied, so the solution exists and is unique. The analytical solution of the inverse problem (2.1)–(2.4) is given by

$$h(t) = 1 + t, \quad u(x,t) = (1+x)^2 + e^t, \tag{5.2}$$

and

$$h(t) = 1 + t, \quad v(y,t) = u(yh(t),t) = (1 + y + yt)^2 + e^t, \tag{5.3}$$

is the analytical solution of the problem (2.6)–(2.9).

We consider the case where there is no noise (i.e. $p = 0$), and then where there is $p = 2\%$ noise in the input data (2.9). The functional (4.3) is represented in Fig. 3, as a function of the number of iterations. 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 (4.3) decreases rapidly and takes a stationary value $O(10^{-7})$ and 0.3411 for $p = 0$ and $p = 2\%$, respectively. The numerical results for the corresponding unknown free boundary $h(t)$ are presented in Fig. 4. The retrieved free boundary $h(t)$ is in very good agreement with the exact one in the case when there is no noise in the input data, while the retrieved solution is stable and within the same range of errors as the input data when it is contaminated by $p = 2\%$ noise. The restored temperatures $v(y,t)$ and $u(x,t)$ for $p = 2\%$ noise are shown in Figs. 5 and 6, respectively. It can be seen that the solutions are stable by being free of

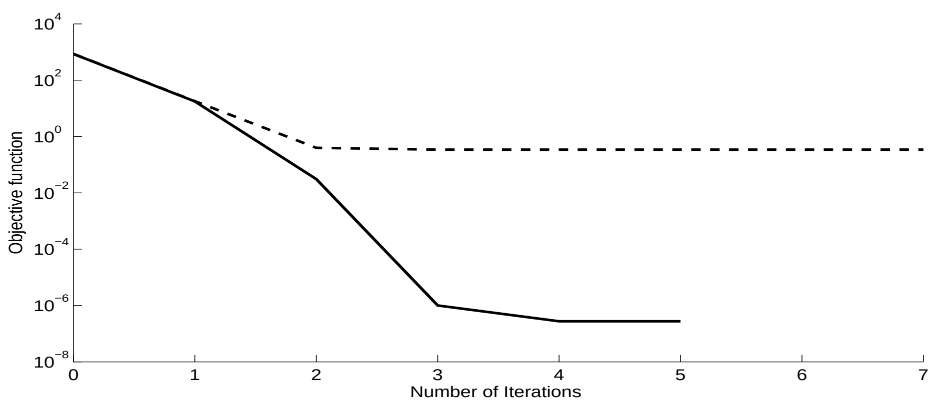

Figure 3: Objective function (4.3) without noise (—), and for $p = 2\%$ noise (- - -) for Example 5.1.

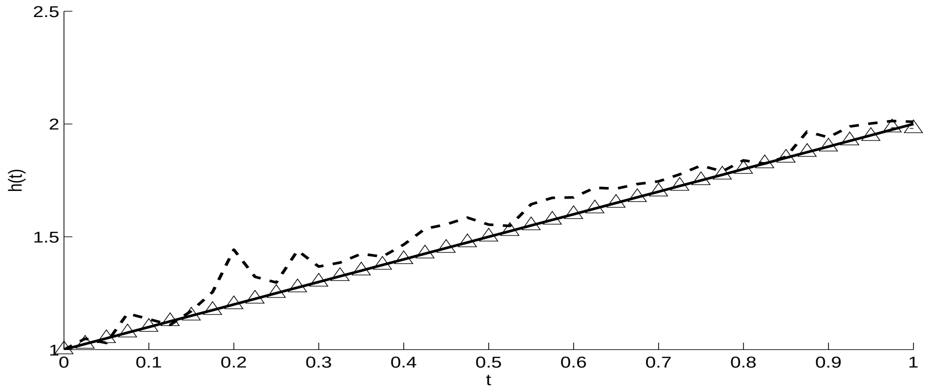

Figure 4: Free boundary $h(t)$, without noise (-△-), and for $p=2\%$ noise (- - -) in comparison with the exact solution (—), for Example 5.1.

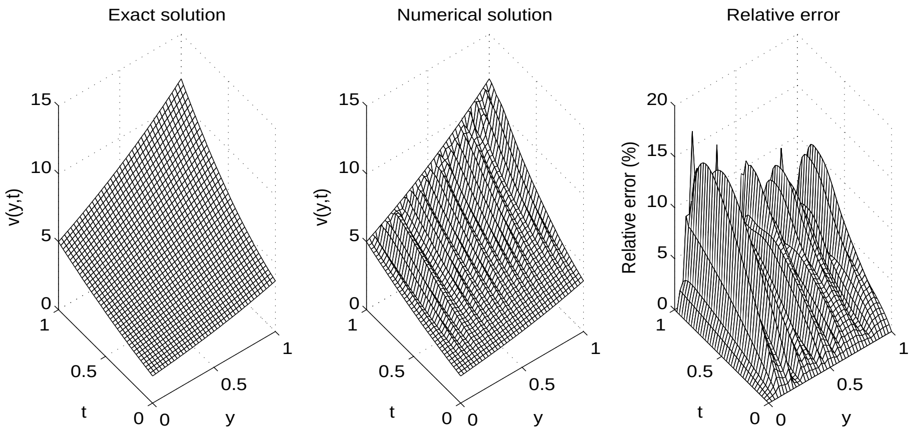

Figure 5: The analytical and numerical solutions, and the relative error for $v(y,t)$ for $p=2\%$ noise for Example 5.1.

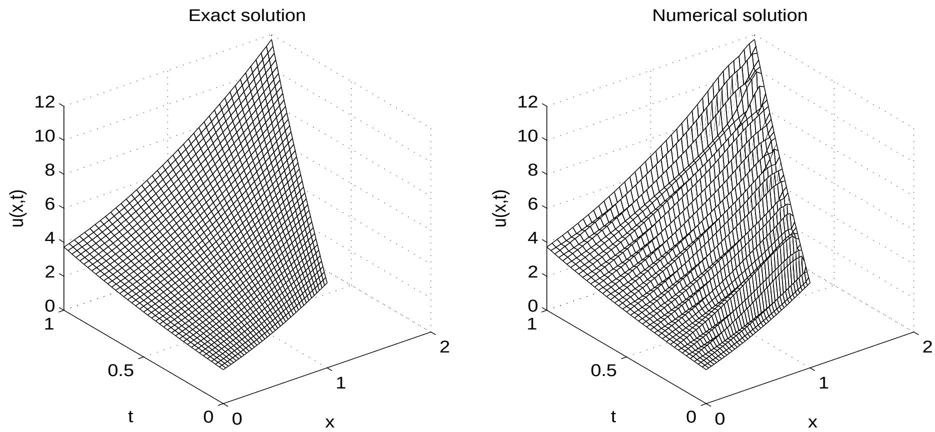

Figure 6: The analytical and numerical solutions for $u(x,t)$ for $p=2\%$ noise for Example 5.1.

high oscillations and unbounded behaviour. Thus for this example it seems that the inverse problem is well-posed and 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 $u(x,t)$.

Example 5.2. We now consider a more severe test case where the unknown function $h(t)$ is nonlinear with the following data

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

The conditions of Theorems 2.1 and 2.2 are satisfied, so the solution exists and is unique. The analytical solution of the inverse problem (2.1)–(2.4) is given by

$$h(t)=\frac{1}{1+t}, \quad u(x,t)=(1+x)^2+e^t, \tag{5.4}$$

and

$$h(t)=\frac{1}{1+t}, \quad v(y,t)=u(yh(t),t)=\left(1+\frac{y}{1+t}\right)^2+e^t, \tag{5.5}$$

is the analytical solution of the problem (2.6)–(2.9).

We study the case of exact and noisy input data in Eq. (2.9). The objective function (4.3) is presented in Fig. 7, as a function of the number of iterations. The functional decreases very fast to stationary values $O(10^{-7})$ and 0.0188 in about 7 and 12 iterations, for $p=0$ and $p=2\%$ noise respectively. The numerical results for the corresponding free boundary $h(t)$ are presented in Fig. 8, where the identified free boundary is in very good agreement with the exact one in the absence of noise, and this outcome is only a little changed when we perturb the input data with $p=2\%$ noise. The numerical solutions for $v(y,t)$ and $u(x,t)$ are shown in Figs. 9 and 10 respectively, in comparison with the exact solutions for $p=2\%$ noise. As in Example 1, stable numerical solutions are obtained. We conclude that the inverse problem is well-posed, since small errors in the measurement in (2.4) cause only small errors in the retrieved pair solution $(h(t),\ u(x,t))$, and we can say that the problem depends continuously on the input data.

For completeness, the number of iterations, the number of function evaluations, the objective function values at final iteration and $rmse(h)$ are given in Table 1, for both Example 5.1 and Example 5.2. It can be seen that accurate and stable numerical solutions are rapidly achieved by the iterative MATLAB toolbox routine *lsqnonlin*.

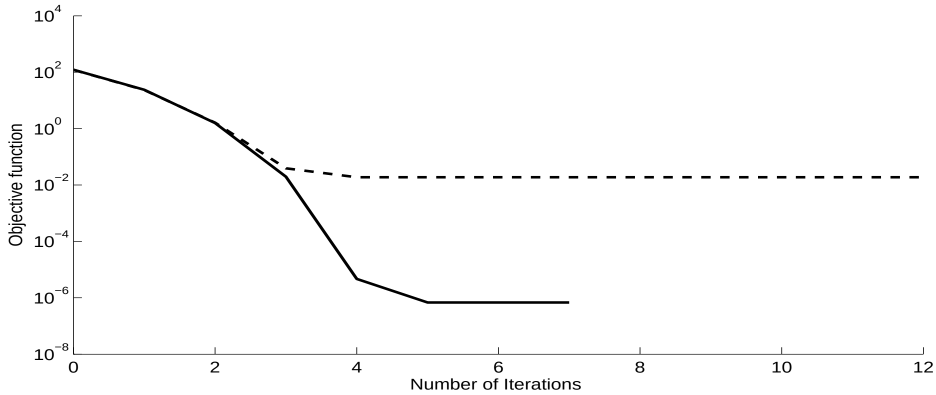

Figure 7: Objective function (4.3) without noise (—), and for $p = 2\%$ noise (- - -) for Example 5.2.

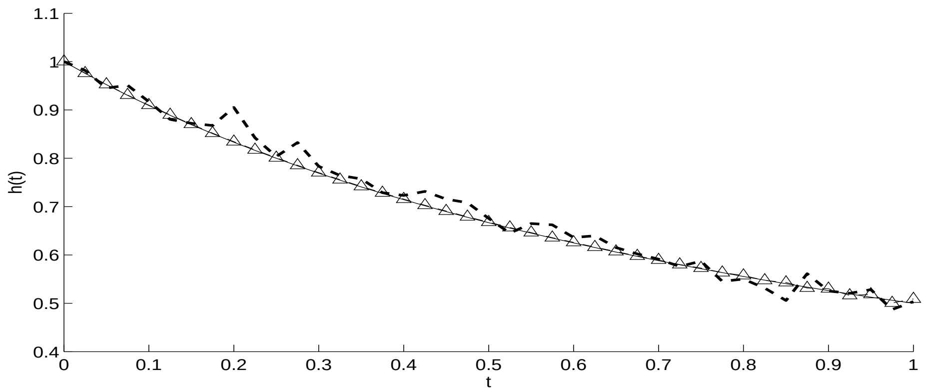

Figure 8: Free boundary $h(t)$, without noise (-△-), and with $p = 2\%$ noise (- - -) in comparison with the exact solution (—), for Example 5.2.

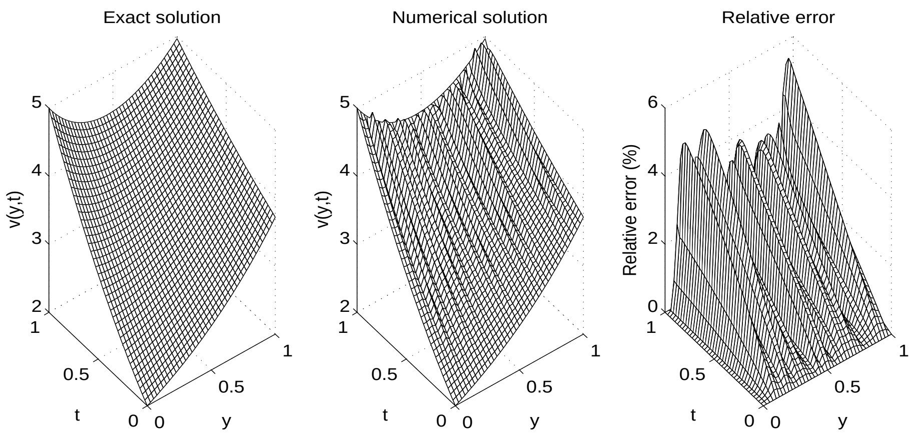

Figure 9: The analytical and numerical solutions and the relative error for $v(y,t)$ for $p = 2\%$ noise for Example 5.2.

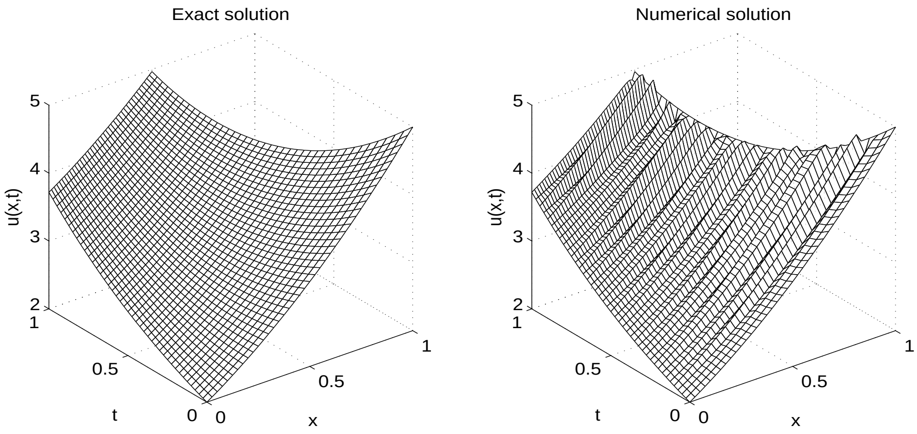

Figure 10: The analytical and numerical solutions for $u(x,t)$ for $p = 2\%$ noise for Example 5.2.

Table 1: Number of iterations, number of function evaluations, value of the objective function (4.3) at final iteration and $rmse$ values (5.1), for Examples 5.1 and 5.2.

		$p = 0$	$p = 2\%$
Example 5.1	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 5.2	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

6. Conclusions

The inverse problem involving identification of the free boundary $h(t)$ and temperature $u(x,t)$ in the heat equation with nonlinear diffusivity $a(u)$ has been investigated. The additional condition that ensures a unique solution is the mass/energy specification $\mu_3(t)$ given by Eq. (2.4). As with other free surface problems, it turns out that the problem is well-posed if the data μ_3 is smooth. A direct solver based on a three-level finite difference scheme is developed. The inverse solver is based on a nonlinear least-squares minimisation, where the MATLAB toolbox routine *lsqnonlin* is used. As expected, the numerical results obtained are very accurate for exact data. For noisy data μ_3^ϵ corresponding to a random perturbation of the exact data μ_3, the results for $h(t)$, $v(y,t)$ and $u(x,t)$ remain stable and accurate. The instability is only manifested in the derivative $h'(t)$, for which the use of a regularisation 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] P. Broadbridge, P. Tritscher and A. Avagliano, *Free boundary problems with nonlinear diffusion*, Math. Comp. Modelling **18**, 15–34 (1993).

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

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

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

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

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

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

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

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

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

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