Zeitschrift für Analysis
und ihre Anwendungen
Bd. 7 (6) 1988, S. 571 – 580

On Parameter Identification for Ordinary Differential Equations

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Es werden Möglichkeiten der regularisierten Lösung von Identifikationsproblemen bei gewöhnlichen Differentialgleichungen für den Fall meßfehlerbehafteter Beobachtungsdaten untersucht. Zur Minimierung der regularisierenden Funktionale werden unter Benutzung des Konzepts der adjungierten Aufgaben sowohl das Gradientenverfahren als auch das Gauß-Newton-Verfahren diskutiert. Eine Anwendung auf eine spezielle inverse Aufgabe der Untersuchung von Untergrundgasspeichern vom Aquifertyp vervollständigt die Arbeit.

Обсуждаются возможности регуляризации решения задач идентификации для обычных дифференциальных уравнений в случае данных содержащих ошибки измерения. Для минимизации регуляризирующего функционала при использовании концепции сопряженной задачи обсуждается применение градиентного метода и метода Гаусса-Ньютона. Дополняет работу применение этой методики к решению одной специальной обратной задачи исследования подземных газовых хранилищ водного типа.

The regularized solution of identification problems in ordinary differential equations is investigated when the data are noisy. For minimizing the occurring regularization functionals the gradient method and the Gauss-Newton method are examined by exploiting the concept of adjoint equations. An application to a particular inverse problem arising in the study of water movement about a gas-storage reservoir of aquifer type completes the paper.

1. Introduction

There has been increasing interest in the identification of parameters in nonlinear ordinary differential equations during the past years. In this paper we are going to discuss particular methods of regularized identification using the concept of adjoint equations. Let us consider the initial value problem

$$\dot{x}(t) = f(t, x, a), \qquad x(0) = x_0, \tag{1.1}$$

where

$$x(t) = \begin{pmatrix} x_1(t) \\ \vdots \\ x_n(t) \end{pmatrix}, \qquad a = \begin{pmatrix} a_1 \\ \vdots \\ a_m \end{pmatrix}, \qquad f(t, x, a) = \begin{pmatrix} f_1(t, x, a) \\ \vdots \\ f_n(t, x, a) \end{pmatrix}.$$

When the data are noisy the regularized parameter identification problem associated with (1.1) can be formulated as follows:

Given noisy observations $z(t) = x(t) + \delta(t)$ $(0 \leqq t \leqq T)$ of the state $x(t)$ $(0 \leqq t \leqq T)$, determine the parameter vector $a \in \mathbf{R}^m$ by minimizing the functional

$$J_\alpha(a) = \frac{1}{2} \|x - z\|_Z^2 + \frac{\alpha}{2} \|a - \bar{a}\|_{R^m}^2 \tag{1.2}$$

over all vectors a of a set $A_{ad} \subset R^m$. Here $x = x_a$ designates the solution of the initial value problem (1.1) *according to* $a \in \mathbf{R}^m$.

The open subset $A_{ad} \subset \mathbf{R}^m$ denotes the set of physically admissible parameters a for which (1.1) has a unique solution $x_a \in X = (C^1[0, T])^n$. Moreover, $Z = (L_2[0, T])^n$ denotes the space of observations, $\bar{a} \in A_{ad}$ is a suitable estimate of the unknown parameters a and α denotes the regularization parameter, which must be chosen appropriately (see e.g. [3]). A number of important identification problems in chemistry (cf. [1, 6]) and other sciences fall within the above framework. An application to the modelling of gas-storage reservoirs of aquifer type is examined in Chapter 3.

Throughout this paper, the norms $\|\cdot\|_Z$ and $\|\cdot\|_{R^m}$ are assumed to be scaled in order to equilibrate the variables. Thus, we will use the norms

$$\|x\|_Z^2 = \sum_{k=1}^{n} \lambda_k \int_0^T x_k^2(t)\, dt \qquad \text{and} \qquad \|a\|_{R^m}^2 = \sum_{k=1}^{m} \varphi_k a_k^2.$$

In this context we introduce a couple of positive definite diagonal matrices

$$\Lambda = \operatorname{diag}(\lambda_k)_1^n \qquad \text{and} \qquad \Phi = \operatorname{diag}(\varphi_k)_1^m.$$

By $(\cdot, \cdot)_Z$ and $(\cdot, \cdot)_{R^m}$ we will denote the inner products in Z and $\mathbf{R}^m$:

$$(x, y)_Z = \sum_{k=1}^{n} \int_0^T x_k(t)\, y_k(t)\, dt \qquad \text{and} \qquad (a, b)_{R^m} = \sum_{k=1}^{m} a_k b_k.$$

The symbols e_i express the unit vectors in $\mathbf{R}^m$.

2. Solution of the minimization problem

In the sequel we will discuss the gradient method and the Gauss-Newton method for the numerical solution of the minimization problem (1.2). For both methods the gradient grad J_α,

$$J_\alpha'(a) \cdot h = \big(\operatorname{grad} J_\alpha(a), h\big)_{R^m} = \lim_{t \to 0} \frac{J_\alpha(a + th) - J_\alpha(a)}{t} \qquad (h \in \mathbf{R}^m)$$

is needed. Let us assume that

(A1) for all $a \in A_{ad}$ the system (1.1) has a unique solution $x \in X$;

(A2) the transformation $H\colon (a, x) \in A_{ad} \times X \to \big(\dot{x} - f(t, x, a), x(0)\big) \in \mathfrak{H}$, $\mathfrak{H} = (C[0, T])^n \times \mathbf{R}^1$, is of $C(A_{ad} \times X, \mathfrak{H})$, i.e. H maps continuously differentiable from $A_{ad} \times X$ into $\mathfrak{H}$;

(A3) for every $(a, x) \in A_{ad} \times X$ the mapping $H_x'(a, x)$ is a linear homeomorphism of X onto $\mathfrak{H}$.

Furthermore, let us introduce the notations

$$F_x' = \begin{pmatrix} \frac{\partial f_1}{\partial x_1} & \cdots & \frac{\partial f_1}{\partial x_n} \\ \vdots & & \vdots \\ \frac{\partial f_n}{\partial x_1} & \cdots & \frac{\partial f_n}{\partial x_n} \end{pmatrix} \qquad \text{and} \qquad F_a' = \begin{pmatrix} \frac{\partial f_1}{\partial a_1} & \cdots & \frac{\partial f_1}{\partial a_m} \\ \vdots & & \vdots \\ \frac{\partial f_n}{\partial a_1} & \cdots & \frac{\partial f_n}{\partial a_m} \end{pmatrix}.$$

Then we can prove the following result.

Theorem 1: *Let the assumptions* (A 1)—(A 3) *be fulfilled. Then*

(i) *the functional* (1.2) *is of* $C(A_{\mathrm{ad}}, \mathbf{R}^1)$, *i.e.* J_α *maps continuously differentiable from* A_{ad} *into* $\mathbf{R}^1$;

(ii) *the gradient* $\operatorname{grad} J_\alpha(a) \in \mathbf{R}^m$ *is given by*

$$\operatorname{grad} J_\alpha(a) = \sum_{i=1}^{m} e_i \int_0^T (y, F_a' e_i)_{\mathbf{R}^n}\, dt + \alpha \Phi(a - \bar{a}), \tag{2.1}$$

where y *is the solution of the adjoint system*

$$L^* y := -\dot{y}(t) - F_x'^*(t)\, y(t) = \Lambda\big(x(t) - z(t)\big), \qquad y(T) = 0, \tag{2.2}$$

and x *is the solution of* (1.1).

Proof: From the Implicit Function Theorem (cf. [10]) we obtain that under the assumptions (A 1)—(A 3) the implicit function $G: a \in A_{\mathrm{ad}} \to x \in X$ is of $C(A_{\mathrm{ad}}, X)$. Hence, $x - z$ is of $C(A_{\mathrm{ad}}, Z)$. It follows that J_α is of $C(A_{\mathrm{ad}}, \mathbf{R}^1)$. Now for an arbitrary variation $\delta a \in \mathbf{R}^m$ one can derive

$$J_\alpha'(a) \cdot \delta a = \big(\Lambda(x - z), \delta x\big)_Z + \alpha\big(\Phi(a - \bar{a}), \delta a\big)_{\mathbf{R}^m}. \tag{2.3}$$

Furthermore, from (1.1) we get

$$L\delta x := \delta\dot{x}(t) - F_x'\delta x(t) = F_a'\delta a, \qquad \delta x(0) = 0. \tag{2.4}$$

Using the initial conditions $y(T) = 0$ and $\delta x(0) = 0$, partial integration yields

$$(y, L\delta x)_Z = (y, \delta\dot{x} - F_x'\delta x)_Z = -(\dot{y} + F_x'^* y, \delta x)_Z = (L^* y, \delta x)_Z. \tag{2.5}$$

Now from (2.3), using (2.2), (2.5) and (2.4) we establish

$$\begin{aligned} J_\alpha'(a) \cdot \delta a &= (L^* y, \delta x)_Z + \alpha\big(\Phi(a - \bar{a}), \delta a\big)_{\mathbf{R}^m} = (y, L\delta x)_Z + \alpha\big(\Phi(a - \bar{a}), \delta a\big)_{\mathbf{R}^m} \\ &= (y, F_a'\delta a)_Z + \alpha\big(\Phi(a - \bar{a}), \delta a\big)_{\mathbf{R}^m} \\ &= (F_a'^* y, \delta a)_Z + \alpha\big(\Phi(a - \bar{a}), \delta a\big)_{\mathbf{R}^m} \\ &= \left(\sum_{i=1}^{m} e_i \int_0^T (F_a'^* y, e_i)_{\mathbf{R}^m}\, dt, \delta a\right)_{\mathbf{R}^m} + \alpha\big(\Phi(a - \bar{a}), \delta a\big)_{\mathbf{R}^m}, \end{aligned}$$

which proves the theorem ∎

Remark: Let us regard the special case of linear systems of ordinary differential equations (1.1) that attain the form

$$\dot{x}(t) = Bx(t) + g(t), \qquad x(0) = x_0. \tag{2.6}$$

Here, the n^2 elements b_{ij} $(i, j = 1, \ldots, n)$ of the matrix B are given functions of the unknown parameter vector $a \in \mathbf{R}^m$. Then the computation of $\operatorname{grad} J_\alpha(a)$ requires

1. the solution of (2.6) in order to find $x = x(t)$,
2. the solution of the adjoint equation

$$-\dot{y}(t) = B^* y(t) + \Lambda\big(x(t) - z(t)\big), \qquad y(T) = 0$$

in order to find $y = y(t)$ and

3. the computation of

$$\operatorname{grad} J_\alpha(a) = \sum_{i=1}^{m} (y, B_i' x)_Z\, e_i + \alpha\Phi(a - \bar{a}),$$

where $B_i' = \partial B / \partial \tilde{a}_i$ can be found from B by elementwise differentiation of B with respect to a_i.

Applying Theorem 1, any iteration step of the gradient method for minimizing (1.2)

$$a^{k+1} = a^k - \gamma_k \operatorname{grad} J_\alpha(a^k), \tag{2.7}$$

requires the solution of one direct problem (1.1), and moreover the solution of one adjoint problem (2.2). Finally, formula (2.1) has to be verified. The parameter γ_k in (2.7) denotes the step length parameter, which must be chosen appropriately. If $a^{k+1} \notin A_{\text{ad}}$, then an additional projection of a^{k+1} into A_{ad} is necessary.

Since such minimization problems (1.2) in general have a flat global minimum in deep banana-shaped valleys, problem (1.2) should better be treated by the Gauss-Newton method which makes it possible to proceed in great steps along the deep valleys and assures fast convergence. Let us denote by $G: a \in A_{\text{ad}} \to x \in X$ the implicit function for the system (1.1). Then in the Gauss-Newton method a given iterate a^k is improved by

$$a^{k+1} = a^k + \gamma_k \Delta a^k, \tag{2.8}$$

where Δa^k is the solution of the linearized functional

$$\|G(a^k) + G'(a^k)\, \Delta a^k - z(t)\|_Z^2 + \alpha\, \|a^k + \Delta a^k - \bar{a}\|_{\mathbf{R}^m}^2.$$

Hence, (2.8) is given by

$$a^{k+1} = a^k - \gamma_k (G'^* \Lambda G' + \alpha \Phi)^{-1} \operatorname{grad} J_\alpha(a^k). \tag{2.9}$$

The computation of G' is the most time-consuming part of the Gauss-Newton iteration (2.9). One way to compute G' is the use of a finite difference approximation G_τ' to the derivative G':

$$G_\tau'(a) = (g^1 \cdots g^i \cdots g^m),$$

$$g^i \in Z, \qquad g^i = \frac{G(a + \tau(a_i)\, e_i) - G(a)}{\tau(a_i)} \qquad (i = 1, \ldots, m),$$

$$|\tau(a_i)| = \tau_{\text{rel}}\, |a_i| + \tau_{\text{abs}}, \qquad \tau_{\text{rel}}, \tau_{\text{abs}} > 0.$$

The derivative $G'(a)$ can thus be approximated by solving the *nonlinear* initial value problem (1.1) $(m + 1)$ times.

The second way to compute $G'(a)$ is the use of the Implicit Function Theorem. If (A 1)–(A 3) are fulfilled, then we have $G' = -H_x'^{-1} H_a'$. In this way there are no problems in choosing τ_{rel} and τ_{abs} appropriately and the amount of computational work is reduced. The route how to compute $G'^* \Lambda G'$ is given in the subsequent

Lemma 1: *Let the assumptions* (A 1)–(A 3) *be fulfilled. Then the* (m, m)*-matrix* $G'^* \Lambda G' = (g_{ij})_1^m$ *can be computed by the following steps:*

(a) *Solve* $\dot{g}^i = F_x' g^i + F_a' e_i$, $g^i(0) = 0 \quad (i = 1, \ldots, m)$; (2.10)

(b) *Compute* $g_{ij} := \int_0^T (g^i, \Lambda g^j)_{\mathbf{R}^n}\, dt$. (2.11)

Remarks: 1. The m initial value problems (2.10) are of the form (2.6). They are linear and can be solved simultaneously. 2. The gradient formula (2.1) is equivalent to

$$\operatorname{grad} J_\alpha(a) = \sum_{i=1}^m e_i \int_0^T (g^i, \Lambda(x - z))_{\mathbf{R}^n}\, dt + \alpha \Phi(a - \bar{a}), \tag{2.12}$$

where the functions g^i are solutions of (2.10).

Using Lemma 1 and Remark 2, one iteration step of the Gauss-Newton method (2.9) requires

(a) the solution of (1.1) in order to find $x = x(t)$,
(b) the simultaneous solution of the m linear initial value problems (2.10),
(c) the computation of grad $J_\alpha'(a)$ by formula (2.12),
(d) the generation of the matrix $G'^*\Lambda G' + \alpha\Phi$ using (2.11) and
(e) the computation of the new iterate $a_{\text{new}} := a - \gamma(G'^*\Lambda G' + \alpha\Phi)^{-1} \operatorname{grad} J_\alpha(a)$.

3. Parameter identification in a particular nonlinear initial value problem

3.1 Mathematical model and properties. Let us consider a one-dimensional gas-storage model of aquifer type characterized by the space domain $[0, L] \subset \mathbf{R}^1$:

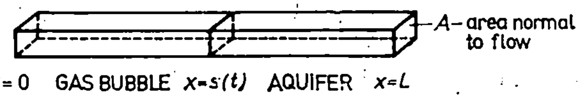

Fig. 1 One-dimensional flow model

We suppose that

(i) the permeability $k_g(x)$ with respect to gas is much greater than the permeability $k_w(x)$ with respect to water,
(ii) the water is incompressible and
(iii) for $t = 0$ and for $x = L$ we have a constant pressure p_0.

Then the physical relations in flow of water and gas through porous media during a time interval $0 \leqq t \leqq T$ are characterized by

$$\frac{\partial}{\partial x}\left(a(x)\,\frac{\partial p_w(x,t)}{\partial x}\right) = 0 \qquad \big(s(t) < x < L,\, 0 \leqq t \leqq T\big), \tag{3.1}$$

$$\eta A s(t)\, p_g(t) = V(t) \qquad \big(0 \leqq x \leqq s(t),\, 0 \leqq t \leqq T\big), \tag{3.2}$$

$$p_g(t) = p_w(x,t) \qquad \big(x = s(t),\, 0 \leqq t \leqq T\big), \tag{3.3}$$

$$p_w(x,t) = p_0 > 0 \qquad (x = L;\, 0 \leqq t \leqq T), \tag{3.4}$$

$$p_g(t) = p_0 > 0 \qquad \big(0 \leqq x \leqq s(0),\, t = 0\big), \tag{3.5}$$

$$-a(x)\,\frac{\partial p_w(x,t)}{\partial x} = c\dot{s}(t) \qquad \big(x = s(t),\, 0 \leqq t \leqq T\big), \tag{3.6}$$

where $a = k_w/\eta_w$ and

η_w — water viscosity,
p_w — pressure in the aquifer,
p_g — pressure in the gas bubble,
η — porosity of medium ($\eta = \text{const}$),
V — amount of gas in the gas bubble under normal pressure.

Equation (3.6) expresses that the water flow rate is proportional to the change of s with respect to the time. An equivalent relation to (3.6) is given in the next Lemma:

Lemma 2: *The equation* (3.6) *can be replaced by the equivalent condition*

$$p_w(s(t), t) = p_0 + c\dot{s}(t) \int_{s(t)}^{L} \frac{d\xi}{a(\xi)}. \tag{3.7}$$

Proof: Owing to formula (3.1) partial integration yields for $p := p_w$ the relation

$$0 = \int_{s(t)}^{L} (ap_x)_x v \, dx = ap_x v \,|_{s(t)}^{L} - pav_x|_{s(t)}^{L} + \int_{s(t)}^{L} (av_x)_x \, p \, dx.$$

Now, setting $v = \int_x^L a(\xi)^{-1} d\xi$, we obtain in view of $v_x = -1/a(x)$ and $(av_x)_x = 0$ the equation

$$0 = -a(s(t)) \, p_x(s(t), t) \int_{s(t)}^{L} \frac{d\xi}{a(\xi)} + p(L, t) - p(s(t), t).$$

Using the boundary condition (3.4), formula (3.6) can be rewritten as (3.7). Thus, we confirm the assertion of the Lemma ∎

From Lemma 2 we see that we can use either (3.6) or (3.7) in deriving properties of the Stefan problem (3.1)—(3.6). Throughout this discussion we assume the existence of a classical solution $(s, p_w) = (s(t), p_w(x, t)) \in C^1[0, T] \times C^{2,0}((s(t), L), [0, T])$ to the Stefan problem (3.1)—(3.6). Furthermore, we will suppose that $L > s(t)$, $a(x) \geqq a_0 > 0$ and $c > 0$.

Lemma 3: *Let* (s_1, p_{w_1}) *and* (s_2, p_{w_2}) *be solutions to the Stefan problem* (3.1)—(3.6) *corresponding to the data* $V_1(t)$ *and* $V_2(t)$ $(0 \leqq t \leqq T)$, *respectively. If* $0 \leqq V_1(t) < V_2(t)$ $(0 \leqq t \leqq T)$, *then* $s_1(t) < s_2(t)$ $(0 \leqq t \leqq T)$.

Proof: Assume the contrary to the assertion and let $t_0 > 0$ be the smallest t for which $s_1(t) = s_2(t)$. Then we have $\dot{s}_1(t_0) \geqq \dot{s}_2(t_0)$. Now from $V_1(t_0) < V_2(t_0)$, (3.2) and (3.3) it follows that $p_{w_1}(s_1(t_0), t_0) < p_{w_2}(s_2(t_0), t_0)$. By using (3.7) we thus have

$$p_0 + c\dot{s}_1(t_0) \int_{s_1(t_0)}^{L} \frac{d\xi}{a(\xi)} < p_0 + c\dot{s}_2(t_0) \int_{s_2(t_0)}^{L} \frac{d\xi}{a(\xi)},$$

hence $\dot{s}_1(t_0) < \dot{s}_2(t_0)$ in contradiction to $\dot{s}_1(t_0) \geqq \dot{s}_2(t_0)$ ∎

Lemma 4: *Let* (s, p_w) *and* (s^δ, p_w^δ) *be solutions to the Stefan problem* (3.1)—(3.6) *corresponding to the data* $V(t)$ *and* $V(t) + \delta$ $(0 \leqq t \leqq T)$, *respectively. If* $\delta > 0$, *then*

$$s^\delta(t)^2 < s(t)^2 + \frac{\delta}{\eta A} \left\{ \frac{2t}{c} + \frac{\delta + 2V(0)}{\eta A p_0^2} \int_{s(t)}^{L} \frac{d\xi}{a(\xi)} \right\} \Bigg/ \int_{s^\delta(t)}^{L} \frac{d\xi}{a(\xi)}.$$

Proof: Multiplying (3.7) by $\eta A s(t)$ and using (3.2) yields

$$V(t) = \eta A p_0 s(t) + c\eta A s(t) \, \dot{s}(t) \int_{s(t)}^{L} \frac{d\xi}{a(\xi)}.$$

Now integration provides

$$\int_0^t V(\tau)\,d\tau = \eta A p_0 \int_0^t s(\tau)\,d\tau + c\eta A \int_{s(0)}^{s(t)} x \left[\int_0^L \frac{d\xi}{a(\xi)} - \int_0^x \frac{d\xi}{a(\xi)}\right] dx.$$

Therefore,

$$\frac{c\eta A}{2} \int_0^L \frac{d\xi}{a(\xi)} [s(t)^2 - s(0)^2]$$

$$= \int_0^t V(\tau)\,d\tau - \eta A p_0 \int_0^t s(\tau)\,d\tau + c\eta A \int_{s(0)}^{s(t)} x \int_0^x \frac{d\xi}{a(\xi)}\,dx.$$

Hence, the solutions (s, p_w) and $(s^\delta, p_w{}^\delta)$ must both satisfy this equation. We subtract those versions and obtain

$$\frac{c\eta A}{2} \int_0^L \frac{d\xi}{a(\xi)} [s^\delta(t)^2 - s(t)^2] = \frac{c\eta A}{2} \int_0^L \frac{d\xi}{a(\xi)} [s^\delta(0)^2 - s(0)^2]$$

$$+ \delta t - \eta A p_0 \int_0^t [s^\delta(\tau) - s(\tau)]\,d\tau + c\eta A \int_{s(t)}^{s^\delta(t)} x \int_0^x \frac{d\xi}{a(\xi)}\,dx$$

$$- c\eta A \int_{s(0)}^{s^\delta(0)} x \int_0^x \frac{d\xi}{a(\xi)}\,dx,$$

where we have used the property

$$\int_{s^\delta(0)}^{s^\delta(t)} \varphi(x)\,dx - \int_{s(0)}^{s(t)} \varphi(x)\,dx = \int_{s(t)}^{s^\delta(t)} \varphi(x)\,dx - \int_{s(0)}^{s^\delta(0)} \varphi(x)\,dx, \qquad \varphi(x) = x \int_0^x \frac{d\xi}{a(\xi)}.$$

From Lemma 3 we have learned that $s^\delta(t) > s(t)$, hence

$$\int_0^L \frac{d\xi}{a(\xi)} [s^\delta(t)^2 - s(t)^2]$$

$$< \int_0^L \frac{d\xi}{a(\xi)} [s^\delta(0)^2 - s(0)^2] + \frac{2\delta t}{c\eta A} + 2 \int_{s(t)}^{s^\delta(t)} x \int_0^x \frac{d\xi}{a(\xi)}\,dx - 2 \int_{s(0)}^{s^\delta(0)} x \int_0^x \frac{d\xi}{a(\xi)}\,dx.$$

Using again $s^\delta(t) > s(t)$ we find

$$\int_0^{s(t)} \frac{d\xi}{a(\xi)} \leqq \int_0^x \frac{d\xi}{a(\xi)} \leqq \int_0^{s^\delta(t)} \frac{d\xi}{a(\xi)} \quad \text{for} \quad x \in [s(t), s^\delta(t)].$$

Therefore we have

$$\int_0^L \frac{d\xi}{a(\xi)} [s^\delta(t)^2 - s(t)^2]$$

$$< \int_{s(t)}^L \frac{d\xi}{a(\xi)} [s^\delta(0)^2 - s(0)^2] + \frac{2\delta t}{c\eta A} + \int_0^{s^\delta(t)} \frac{d\xi}{a(\xi)} [s^\delta(t)^2 - s(t)^2],$$

which yields the expected inequality ∎.

Now we are able to prove a more general monotonicity theorem.

Theorem 2: *Let* (s_1, p_{w_1}) *and* (s_2, p_{w_2}) *be solutions to the Stefan problem* (3.1)—(3.6) *corresponding to the data* $V_1(t)$ *and* $V_2(t)$ $(0 \leqq t \leqq T)$, *respectively. If* $0 \leqq V_1(t) \leqq V_2(t)$, *then* $s_1(t) \leqq s_2(t)$ $(0 \leqq t \leqq T)$.

Proof: For $\delta > 0$, let $(s_2^\delta, p_{w_2}^\delta)$ be solutions to the Stefan problem (3.1)—(3.6) corresponding to the data $V_2(t) + \delta$. From Lemma 3 we see that $s_1 < s_2^\delta$. Using Lemma 4 we find

$$s_1(t)^2 < s_2(t)^2 + \frac{\delta}{\eta A} \left\{\frac{2t}{c} + \frac{\delta + 2V_2(0)}{\eta A p_0^2} \int_{s_2(t)}^L \frac{d\xi}{a(\xi)}\right\} \Big/ \int_{s_2^\delta(t)}^L \frac{d\xi}{a(\xi)}.$$

Since $\delta > 0$ can be chosen as small as desired, it follows that $s_1(t) \leqq s_2(t)$ ∎

As a corollary of Theorem 2 we obtain the following uniqueness theorem.

Theorem 3: *The solution* (s, p_w) *to the Stefan problem* (3.1)—(3.6) *is uniquely determined.*

Proof: If (s_1, p_{w_1}) and (s_2, p_{w_2}) both correspond to the data $V(t)$, $0 \leqq t \leqq T$, then from Theorem 2 we have $s_1 \leqq s_2$ and $s_2 \leqq s_1$, which implies that $s_1 = s_2$. Therefore we have $\dot{s}_1 = \dot{s}_2$. Now using (3.7) we obtain $p_{w_1}(s_1(t), t) = p_{w_2}(s_1(t), t)$ $(0 \leqq t \leqq T)$. Owing to (3.4) and (3.1) this provides $p_{w_1} = p_{w_2}$ ∎

3.2 The identification problem. The identification of the unknown function $a = a(x)$, $0 \leqq x \leqq L$, from measured field data values $V(t)$ and $p_g(t)$ $(0 \leqq t \leqq T)$ is of great practical importance. In order to realize this aim it suffices to consider the free boundary $x = s(t)$. Owing to (3.2), (3.3) and (3.7) we have

$$p_g(t) = p_0 + c\dot{s}(t) \int_{s(t)}^L \frac{d\xi}{a(\xi)} \qquad (0 \leqq t \leqq T). \tag{3.8}$$

We assume that there are given functions φ_i, $\varphi_i(x) > 0$ $(0 \leqq x \leqq L; i = 1, 2, \ldots, m)$ such that

$$\big(a(x)\big)^{-1} = \sum_{i=1}^m a_i\varphi_i(x) \qquad (a_i \geqq 0, i = 1, 2, \ldots, m).$$

Moreover, let us suppose that the antiderivatives of φ_i possess a simple structure such that $\psi_i(\tau) = \int_\tau^L \varphi_i(\xi)\, d\xi$ $(0 \leqq \tau \leqq L; i = 1, 2, \ldots, m)$ is explicitly available. Then (3.8) may be rewritten as

$$p_g(t) = p_0 + c\dot{s}(t) \sum_{i=1}^{m} a_i \psi_i(s(t)) \qquad (0 \leqq t \leqq T).$$

For given positive values η, A, p_0, $v_0 = V(0)$ the initial value $s(0) = s_0 = v_0/(p_0 \eta A)$ is determined. Thus, the initial value problem

$$\dot{s}(t) = f(t, s, a) := \frac{p_g(t) - p_0}{c \sum_{i=1}^{m} a_i \psi_i(s(t))}, \qquad s(0) = s_0 \tag{3.9}$$

attains the form (1.1) with $n = 1$. The noisy observations $z(t) = s(t) + \delta(t)$ $(0 \leqq t \leqq T)$ are won from noisy measurements $z_1(t) = V(t) + \delta_1(t)$ $(0 \leqq t \leqq T)$ and $z_2(t) = p_g(t) + \delta_2(t)$ $(0 \leqq t \leqq T)$ by the formula (cf. (3.2)) $z(t) = z_1(t)/(\eta A z_2(t))$. When a fixed vector $a \in A_{ad} = \{\bar{a} \in \mathbf{R}^m : \bar{a}_i \geqq 0 \ (i = 1, 2, \ldots, m)\}$ is considered, then in view of Theorem 3 the direct problem (3.9) is uniquely solvable. On the other hand, the inverse problem of estimating $a \in A_{ad}$ from the data z may be realized by regularized parameter identification (see (1.2)). Then

$$J_\alpha(a) = \frac{1}{2} \|s - z\|^2_{L_2[0,T]} + \frac{\alpha}{2} \|a - \bar{a}\|^2_{\mathbf{R}^m}$$

is to be minimized over $a \in A_{ad}$. However, the solutions $s = s_a$ of (3.9) are in practice also perturbed. Namely, the values $f(t, s, a)$ must be replaced by $\tilde{f}(t, s, a) = (z_2(t) - p_0) / \left(c \sum_{i=1}^{m} a_i \psi_i(s(t))\right)$. Thus, this additional error is to be taken into consideration when a discrepancy principle for choosing the regularization parameter $\alpha > 0$ is used.

Acknowledgement. The author is grateful to Prof. Dr. B. Hofmann for several remarks and constructive comments that contributed to the finished form of the paper.

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Manuskripteingang: 24. 11. 1987

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