PARAMETER IDENTIFICATION IN REACTION-DIFFUSION MODELS

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Abstract. We consider certain one-dimensional reaction-diffusion models for two chemical substances with concentrations A ("the reducing agent") and B ("the coupler"). The reducing agent diffuses and combines with the coupler. Both the diffusion coefficient D and the reaction rate k are unknown. The measurable quantity is the total concentration $h(t)$ of the reducing agent, or its concentration $g(t)$ at the wall of the container, at each time t. The problem is therefore to identify D and k from the knowledge of h or g. An asymptotic expansion of A for small times reveals the dependence of $h(t)$ and $g(t)$ on D and k thereby allowing us to identify these coefficients.

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1. Statement of the problems. In this section we consider two reaction diffusion models which arise in color negative film development [1; Chap 10]. The first problem is modelled as follows:

$$\frac{\partial A}{\partial t} = D\frac{\partial^2 A}{\partial x^2} - kAB \qquad (0 < x < L\ ,\ t > 0)\ , \tag{1.1}$$

$$\frac{\partial B}{\partial t} = -kAB \qquad (0 < x < L\ ,\ t > 0) \tag{1.2}$$

with

$$A(x,0) = 1 \qquad (0 < x < L)\ , \tag{1.3}$$

$$B(x,0) = 1 \qquad (0 < x < L)\ , \tag{1.4}$$

$$\frac{\partial A}{\partial x}(L,t) = 0 \qquad (t > 0) \tag{1.5}$$

and

$$A(0,t) = 0 \qquad (t > 0)\ . \tag{1.6}$$

Here A and B are the concentrations of two chemical substances, the reducing agent and the coupler (oil droplets). The diffusion coefficient and the reaction rate k are not known. One measures the total concentration

$$h(t) = \int_0^L A(x,t)dx \tag{1.7}$$

and wishes to use this information in order to determine D and k.

In the second model, we have the same differential equations (1.1), (1.2). The conditions (1.4), (1.5) are also the same but (1.3) and (1.6) are replaced by

$$A(x,0) = 0 \qquad (0 < x < L) \tag{1.3'}$$

and

$$\begin{cases} A(0,0+) = 1\ , \\ \dfrac{\partial A}{\partial t}(0,t) = -D\dfrac{\partial A}{\partial x}(0,t) \qquad (t > 0)\ . \end{cases} \tag{1.6'}$$

We can rewrite (1.6′) in the form

$$A(0,t) = 1 - \int_0^t D\frac{\partial A}{\partial x}(0,s)ds\,. \tag{1.6″}$$

Here the measured quantity is the concentration of A at $x = 0$:

$$g(t) = A(0,t) = 1 - \int_0^t D\frac{\partial A}{\partial x}(0,s)ds \tag{1.8}$$

and we wish to determine the unknown coefficients D and k.

DEFINITION 1.1. The system (1.1)–(1.6) will be called (S), and the identification problem of determining D and k from the knowledge of the function h in (1.7) will be called (IS). Similarly, we define the system (S') and the identification problem (IS') for the system (1.1), (1.2), (1.3′), (1.4), (1.5), (1.6″) with data given by (1.8).

For the background material on these two problems we refer to [2].

In §2 we solve the problem (IS) and in §3 we solve (IS').

2. Solution of the problem (IS). Clearly

$$B(x,t) = e^{-k\int_0^t A(x,s)ds}$$

so that (1.1), (1.2), (1.4) can be reduced to

$$A_t = DA_{xx} - kAe^{-k\int_0^t A(x,s)ds}\,. \tag{2.1}$$

To study the system (2.1), (1.3), (1.5), (1.6) we observe that A has a discontinuity at $x = t = 0$. In order to prove existence and uniqueness and further analyze the behavior of the solution near (0,0), we introduce the function

$$w(x,t) = \frac{2}{\sqrt{\pi}}\int_0^{x/\sqrt{4Dt}} e^{-\rho^2}d\rho$$

and set

$$A = w - ktw + ku\,. \tag{2.2}$$

Note that

$$w_x(x,t) = \frac{2}{(4\pi Dt)^{1/2}}\ e^{-x^2/(4Dt)}\ ,$$

$$w_t(x,t) = \frac{-x}{(4\pi D)^{1/2} t^{3/2}}\ e^{-x^2/(4Dt)}\ ,$$

$$w_t = Dw_{xx} \qquad (x > 0\ ,\ t > 0)$$

and

$$w(0,t) = 0\ ,\ w(x,0) = 1 \qquad (x > 0\ ,\ t > 0)\ .$$

Hence, the system (S) reduces to

$$u_t - Du_{xx} = k(tw - u)e^{-k\int_0^t (w - ktw + ku)} + w\left(1 - e^{-k\int_0^t (w-ktw+ku)}\right), \tag{2.3}$$

$$u(0,t) = 0 \qquad (t > 0)\ , \tag{2.4}$$

$$u_x(L,t) = \left(t - \frac{1}{k}\right) w_x(L,t) \qquad (t > 0) \tag{2.5}$$

and

$$u(x,0) = 0 \quad (0 < x < L). \tag{2.6}$$

Observe that the right and side of (2.5) tends to zero (together with its derivatives) as t approaches zero, so that the lateral data is compatible with the initial condition.

THEOREM 2.1. *There exists a unique solution u of (2.3)–(2.6) in $C^{3+\beta}([0,L] \times [0,T])$, for all $0 < \beta < 1\ ,\ T > 0$.*

Here $C^{3+\beta}$ is a Hölder space taken in the parabolic sense (see [3;p. 7]) so that $u_{xt}\ ,\ u_{xxx}$ are in $C^{\beta,\beta/2}_{x,t}$.

Proof. We use a fixed point argument in the space $C^{1+\beta}([0,L] \times [0,\tau])$. Given $u \in C^{1+\beta}$, denote the right hand side of (2.3) by $F(u)$ and the solution of

$$\overline{u}_t - D\overline{u}_{xx} = F(u)$$

subject to the conditions (2.4)–(2.6) by $\overline{u}$. Set $\overline{u} = \mathcal{R}u$. Then ([3; Chap IV]) $\mathcal{R}$ is a mapping from $C^{1+\beta}$ into $C^{3+\beta}$. Further,

$$\|\mathcal{R}u\|_{C^{1+\beta}} \leq c_1 \tau^{\frac{1-\beta}{2}}\ \|u\|_{C^{1+\beta}} + c_2$$

and

$$\|\mathcal{R}u_1 - \mathcal{R}u_2\|_{C^{1+\beta}} \le c_0 \tau^{\frac{1-\beta}{2}} \|u_1 - u_2\|_{C^{1+\beta}}$$

for some constants c_0, c_1, c_2 independent of u, u_1 and u_2.

It follows that, for small τ, $\mathcal{R}$ is a contraction, and thus the system (2.3)–(2.6) has a unique solution. Since A is a priori bounded (by the maximum principle), we can extend the solution uniquely step-by-step to any interval $[0, T]$. □

Observe that

$$h(t) = \int_0^L A(x,t)dx = \int_0^L w - k \int_0^L tw + k \int_0^L u \ ,$$

so that

$$h'(t) = -\frac{\sqrt{D}}{\sqrt{\pi t}}\left(1 - e^{-L^2/(4Dt)}\right) + O(1) \quad \text{as} \quad t \to 0 \tag{2.7}$$

and

$$h''(t) - \int_0^L w_{tt}(x,t)dx = \frac{k\sqrt{D}}{\sqrt{\pi t}}\left\{\frac{1}{2} - \frac{1}{2}e^{-L^2/(4Dt)}\left(1 + \frac{L^2}{2Dt}\right)\right\} + k\int_0^L u_{tt}(x,t)dx \, . \tag{2.8}$$

Using (2.7), we see that h determines D. Thus the function w is known and we can use it in (2.8) to determine the reaction rate k since (by Theorem 2.1) the last term on the right hand side of (2.8) remains bounded as $t \to 0$.

We conclude

THEOREM 2.2. *The function $h(t)$ (t small) determines uniquely D and k by the formulae (2.7), (2.8).*

3. Solution of the problem (IS'). We proceed as in §2 but, instead of (2.2), we write

$$A = 1 - w + D\int_0^t w_x(x,s)ds + ktw + u \ . \tag{3.1}$$

Note that the term $\int_0^t w_x$ is in $W_\infty^{1,1/2}$ and the term ktw is in $W_\infty^{2,1}$. Writing

$$u = A - 1 + w - D\int_0^t w_x - ktw$$

we find that

$$u_t - Du_{xx} = -k(1 + D\int_0^t w_x + ktw + u)e^{-k\int_0^t(1-w+D\int_0^s w_x+ksw+u)ds} \tag{3.2}$$
$$+kw(e^{-k\int_0^t(1-w+D\int_0^s w_x+ksw+u)ds} - 1)\ .$$

Further we easily compute that

$$u(0,t) = -D\int_0^t (u_x(0,s) + ksw_x(0,s) - 1)ds \tag{3.3}$$

and also

$$u_x(L,t) = w_x(L,t) - Dw(L,t) + D - ktw_x(L,t)\ , \tag{3.4}$$

$$u(x,0) = 0\ . \tag{3.5}$$

Noticing that the initial and boundary conditions satisfy the compatibility condition, we can establish the following result.

THEOREM 3.1. *There exists a unique solution $u \in C^{2+\beta}$ to (3.2)–(3.5), for any $0 < \beta < 1$.*

Proof. We again use a fixed point argument in $C^{1+\beta}$, as in the proof of Theorem 2.1. □

We now proceed to solve the identification problem (IS'). From (1.8) and (3.1) we deduce that

$$g'(t) = A_t(0,t) = Dw_x(0,t) + u_t(0,t) = \frac{D^{1/2}}{(\pi t)^{1/2}} + O(1) \quad \text{as} \quad t \to 0\ , \tag{3.6}$$

so that once again we can determine D and therefore also the function $w(x,t)$.

Finally, to find k, we use the equality (cf. (1.8))

$$g''(t) = -DA_{xt}(0,t)$$

to write, using (3.1),

$$g''(t) - Dw_{xt}(0,t) + Dw_t(0,t) = -\frac{kD^{1/2}}{2(\pi t)^{1/2}} - Du_{xt}(0,t) \tag{3.7}$$

and observe that this equation determines k since, by (3.2) and Theorem 3.1,

$$\sqrt{t}\, u_{xt}(0,t) \to 0 \quad \text{as} \quad t \to 0 \; .$$

THEOREM 3.2. *The function $g(t)$ (t small) determines uniquely D and k by (3.6) and (3.7).*

REMARK 3.1. From the formulae (2.2) and (3.1) one may easily derive sensitivity (or stability) estimates. For example for (IS'), equation (3.1) implies that, for measurements $g_1(t)$ and $g_2(t)$ corresponding to diffusion coefficients D_1 and D_2 respectively, we have

$$|D_1^{1/2} - D_2^{1/2}| = \left(\frac{\pi}{4t}\right)^{1/2} |g_1(t) - g_2(t)| + O(t^{1/2}) \quad \text{as} \quad t \to 0 \; .$$

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