Parameter Estimation Problem for a Nonlinear Parabolic Equation with a Singular Nonlocal Diffusion Term*

Azmy S. Ackleh†
Department of Mathematics
University of Southwestern Louisiana
Lafayette, Louisiana 70504-1010, USA

Abstract

We study a quasilinear reaction-diffusion problem that models the dynamics of a population that is eager to quickly get out of zones with low population densities. A least squares technique for identifying the singular diffusion coefficient is developed. Numerical results indicating the feasibility of this approach are presented.

Keywords: Parameter identification, quasilinear nonlocal parabolic equation, singular diffusion coefficient.

1 Introduction

We consider the reaction-diffusion problem

$$\begin{cases} u_t = \frac{1}{a(P(t))}u_{xx} + uF(u) & (t,x) \in (0,T] \times (0,1), \\ u(t,0) = 0 = u(t,1) & t \in (0,T], \\ u(0,x) = u^0(x) & x \in [0,1], \end{cases} \tag{1.1}$$

where $P(t) = \int_0^1 u(t,x)dx$. The diffusion coefficient in (1.1) depends on the total population P in the domain. If the function a is an increasing function with $a(0) = 0$ (e.g. $a(P) = P$) then a diffusion of this type models a population that is anxious to quickly move out of territories with low population densities. The term $uF(u)$ describes the reaction or growth of the population. Two commonly used reaction terms are the logistic model where $F(u) = r(C-u)$ and the Monod kinetics where $F(u) = r/(C+u)$ (e.g. Ackleh *et al.*, 1998; Bear, 1972; Freeze and Cherry, 1979; Pao 1992).

Recently, existence-uniqueness of solutions for the homogeneous diffusion problem given by (1.1) with $F(u) = 0$ was established by Chipot and Lovat (1999). In (Ackleh and Ke,

*Research supported in part by the Louisiana Education Quality Support Fund under grant # LEQSF(1996-99)-RD-A-36.

†E-mail: ackleh@usl.edu. The travel to present this paper was partially supported by the Louisiana Board of Regents through a Travel Grant for Emerging Faculty.

1999) this existence-uniqueness result was extended to the reaction-diffusion problem (1.1). Furthermore, the long time behavior of (1.1) with Logistic and Monod type of reaction functions was discussed therein. In particular, the authors established conditions on the initial distribution under which the population becomes extinct in finite time and conditions under which the population approaches a steady state. In this note we continue the investigation of problem (1.1). The main goal here is to develop a numerical method for identifying the function a from observation data.

Several researchers developed an abstract approximation framework for parameter identification problems involving quasilinear parabolic evolution equations (Ackleh *et al.*, 1998; Ackleh and Reich, 1998; Banks *et al.*, 1991, Banks *et al.*, 1990). However, the theories in these papers do not apply to the singular nonlocal diffusion given in (1.1). This paper is organized as follows. In Section 2, a least squares approach for identifying the function $a(P)$ in (1.1) from observation data is developed. Section 3 is devoted to numerical results while in Section 4 some concluding remarks are made.

2 Parameter estimation problem

Consider the following inverse problem: Given observations Z_r which correspond to the total number of individuals in the population at times $t_r \in [0,T]$, $r = 1, 2, \cdots, R$, find a parameter $a \in Q$ which minimizes the least squares cost functional

$$J(a) = \sum_{r=1}^{R} |P(t_r; a) - Z_r|^2 \tag{2.1}$$

where $P(t;a)$, the total number of individuals at time t, is obtained from integrating the parameter dependent solution $u(t,x;a)$ to (1.1) over the interval $(0,1)$. We note that defining the linear operator $Av = v''$ with domain $D(A) = \{v \in H_0^1(0,1) : Av \in L^2(0,1)\}$ then there exists a $t_0 > 0$ such that (1.1) has a unique nonnegative solution $u \in C([0,t_0]; D(A)) \cap C^1((0,t_0); L^2(0,1))$ provided that the following conditions are satisfied (Ackleh and Ke, 1999):

1. The function $F(u)$ is locally Lipschitz continuous.
2. The function $a(P)$ is locally Lipschitz continuous satisfying $a(P) > 0$ for all $P \neq 0$, and $a(0) \geq 0$.
3. $u^0 \in D(A)$ is nonnegative function with $u^0 \neq 0$.

For the rest of our discussion, we let $D = C_B[0,\infty)$ be the space of bounded uniformly continuous functions on $[0,\infty)$, and for fixed positive constants A_1, A_2, $\bar{P}$, and ϵ we choose the admissible parameter set Q to be the D closure of the following set

$$\{a \in C_B[0,\infty) \ : a(0) = 0, \ \epsilon P \leq a(P) \leq A_1 \text{ for } P \in [0,\bar{P}], \ |a'(P)| \leq A_2,$$
$$a(P) = a(P_a) \text{ (i.e., } a \text{ is a constant function) for } P \geq P_a, \text{ where } P_a \leq \bar{P}\}.$$

Using Arzela-Ascoli theorem one can verify that Q is a compact subset of D. The first step in solving the least squares problem is the approximation of (1.1), which we set up using the following implicit finite difference scheme:

$$\begin{cases} \dfrac{u_j^{k+1}-u_j^k}{\Delta t} = \dfrac{1}{a(P^k)}\dfrac{u_{j+1}^{k+1}-2u_j^{k+1}+u_{j-1}^{k+1}}{\Delta x^2} + u_j^{k+1}F(u_j^k) & \begin{array}{c} j=1,\cdots,N-1, \\ k=0,\cdots,L-1 \end{array} \\ u_0^{k+1} = 0 = u_N^{k+1} & k=0,\cdots,L-1 \\ P^{k+1} = \sum_{j=1}^{N-1}\Delta x u_j^{k+1} & k=0,\cdots,L-1 \\ u_j^0 = u^0(x_j) & j=0,\cdots,N \end{cases} \tag{2.2}$$

where $\Delta t = T/L$, $\Delta x = 1/N$, and u_j^k is the finite difference approximation of $u(t,x)$. Hence, solving the discrete system (2.2) is equivalent to solving the following tridiagonal system of linear equations

$$A^k \overrightarrow{u}^{k+1} = \overrightarrow{u}^k \text{ for } k = 0,\ldots,L-1, \tag{2.3}$$

where

$$A^k = \begin{pmatrix} d_1^k & -\dfrac{\mu}{a(P^k)} & 0 & 0 & \cdots & 0 \\ -\dfrac{\mu}{a(P^k)} & d_2^k & -\dfrac{\mu}{a(P^k)} & 0 & \cdots & 0 \\ 0 & -\dfrac{\mu}{a(P^k)} & d_3^k & -\dfrac{\mu}{a(P^k)} & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & \cdots & 0 & -\dfrac{\mu}{a(P^k)} & d_{N-2}^k & -\dfrac{\mu}{a(P^k)} \\ 0 & \cdots & 0 & 0 & -\dfrac{\mu}{a(P^k)} & d_{N-1}^k \end{pmatrix},$$

$$\mu = \frac{\Delta t}{(\Delta x)^2},\ \overrightarrow{u}^{k+1} = \left[u_1^{k+1}, u_2^{k+1}, \ldots, u_{N-1}^{k+1}\right],$$

and

$$d_j^k = 1 - \Delta t F(u_j^k) + \frac{2\mu}{a(P^k)},\ j = 1,\ldots,N-1.$$

Assuming that there exists a constant $E > 0$ such that $F(u) \leq E$ for all $u \geq 0$ then one can verify that the difference approximation has a local nonnegative solution provided that Δt is chosen sufficiently small. Note that this condition is satisfied for the logistic and the Monod reaction terms.

The above approximation can be extended to a function on $[0,1]\times[0,T]$ by defining

$$U_{\Delta t,\Delta x}(t,x;a) = u_j^k(a),\ (t,x)\in(t_{k-1},t_k]\times(x_{j-1},x_j],\ k=1,...,L,\ j=1,...,N$$

where $u_j^k(a)$ denote the parameter dependent solution of equation (2.3). Since our parameter set is infinite dimensional a finite dimensional approximation is necessary for computing minimizers. To this end, we consider the following finite dimensional approximate inverse problem: Given observations Z_r which correspond to the total number of individuals in the population at times $t_r \in [0,T]$, $r = 1,2,\cdots,R$, find a parameter $a \in Q_M$ which minimizes the following approximate cost functional

$$J_{\Delta t,\Delta x}(a) = \sum_{r=1}^{R} |P^{\Delta t,\Delta x}(t_r;a) - Z_r|^2. \tag{2.4}$$

Here, $P^{\Delta t,\Delta x}(t_r;a) = \int_0^1 U_{\Delta t,\Delta x}(t_r,x;a)dx$ and $Q_M = I_M(Q)$, where for each $a \in Q$,

$$(I_M a)(P) = \sum_{i=1}^{M} a\left(\frac{iP_a}{M}\right)\lambda_M^i(P;P_a)$$

where $\lambda_M^i(P;P_a)$, $i = 0,1,\ldots,M$, represent the linear B-splines defined by using the uniform mesh $\{0, \frac{P_a}{M}, \ldots, P_a\}$, on the interval $[0,P_a]$. The function $(I_M a)(P)$ is extended to a continuous function over $[0,\infty)$ by setting $\lambda_M^i(P;P_a) = \lambda_M^i(P_a;P_a)$ for any $P \geq P_a$. The Peano Kernel Theorem is used to yield

$$\lim_{M\to\infty} I_M(a) = a \quad \text{in } C_B[0,\infty),$$

uniformly in a, for $a \in Q$ (Schultz, 1973). Hence, if $a_M \in Q_M = I_M(Q)$ is given by

$$a_M(P) = \sum_{i=1}^{M} \alpha_M^i \lambda_M^i(P;P_a),$$

then the solution of our finite dimensional identification problem involves identifying the $(M+1)$ coefficients $\{\alpha_M^i, P_a\}_{i=1}^M$ from a compact subset of $\mathbb{R}^{M+1}$ so as to minimize the least squares cost functional (2.4).

3 Numerical results

In this section we test the above technique using computationally generated data with random noise. To generate data we choose the parameter functions

$$u^0(x) = 1.5\sin\pi x,\ F(u) = 10 - u, \text{ and } a(P) = 0.9(1 - \exp(-10P^2)),$$

and solve the system of equations (2.3) using $\Delta x = 10^{-2}$ and $\Delta t = 10^{-3}$. Then we let $Z_r = P^{\Delta t,\Delta x}(t_r)$, $t_r = r\Delta t$, $r = 1,2,\ldots,500$. In Figure 1 we present the total population data Z_r as a function of t. Observe that for this choice of parameters, the population is driven to extinction at $t = 0.48$.

To identify the parameter $a(P)$, we used the technique presented in Section 2 with $M = 10$. Hence, our finite dimensional identification problem involved estimating the 11 constants $\{\alpha_{10}^i, P_a\}_{i=1}^{10}$. Rather than implement compactness constraints directly, we work with a regularized cost functional

$$J^\gamma_{\Delta t,\Delta x}(a) = J_{\Delta t,\Delta x}(a) + \gamma\int_0^{\bar{P}} |a'(P)|^2 dP.$$

The properties of the regularized cost functional is examined in details in (Banks and Kunisch, 1989). The compactness of the embedding $H^1(0,\bar{P}) \hookrightarrow C[0,\bar{P}]$ enforces the constraints indirectly. We used LMDIF1 routine obtained from NETLIB that implements the Levenberg-Marquardt algorithm for the minimization.

In Figure 2 we present the difference between the exact function $a(P)$ and the linear spline least squares estimate $a_M(P)$. In this experiment the regularization parameter used $\gamma = 3\times10^{-4}$ and the least squares value obtained $J_{\Delta t,\Delta x}(a_M) = 9\times10^{-5}$. We then modify the data set using noise with mean zero and standard deviation $\sigma = 0.03$ and present the function $a(P)$ versus the linear spline least squares estimate $a_M(P)$ in Figure 3. We use the same regularization parameter as in the previous experiment, and we obtain the least squares value $J_{\Delta t,\Delta x}(a_M) = 0.15$. We note that the mean of the difference between the exact and estimated functions is approximately zero for both of these experiments.

For our second example, we use the function $a(P) = 0.7\frac{P}{0.05+P}$ and generate data using the same procedure discussed above. In Figure 4 we present the total population data versus time. For this choice of the function a, the total population is driven to extinction at $t = 0.43$. In Figure 5 we present the difference between the exact and estimated functions when no noise is added to the data. The least squares value $J_{\Delta t,\Delta x}(a_M)$ for this experiment is 1.3×10^{-3} and the regularization parameter used is $\gamma = 3 \times 10^{-3}$. Finally, in Figure 6 we present the estimated versus the exact function for noisy data with mean zero and standard deviation $\sigma = 0.03$. The regularization parameter used is $\gamma = 3 \times 10^{-2}$ and the final least squares value $J_{\Delta t,\Delta x}(a_M) = 5.9 \times 10^{-2}$.

4 Concluding remarks

The least squares technique developed in this paper appears to be promising for identifying the diffusion coefficient in (1.1). The main focus in this paper was the numerical implementation of this technique. Our future efforts will focus on theoretical questions concerning the convergence of the finite difference approximation (2.2) to the unique solution of problem (1.1). Furthermore, we will investigate the convergence of computed minimizers of the finite dimensional least squares problem (2.4) to a minimizer of the infinite dimensional least squares problem (2.1). A crucial step in obtaining such a result is proving the uniform (in the parameter) convergence of the finite difference approximation (Banks and Kunisch, 1989).

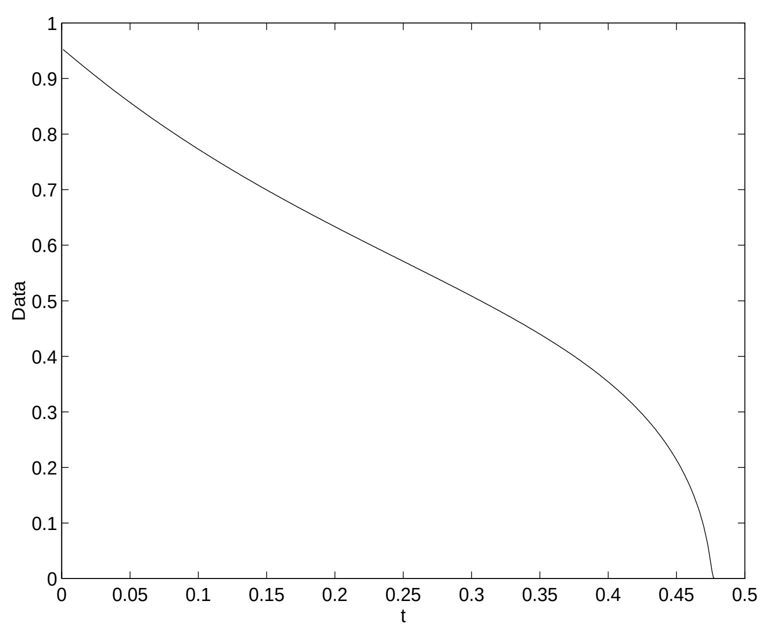

Figure 1: The computationally generated data with $a(P) = 0.9(1 - \exp(-10P^2))$.

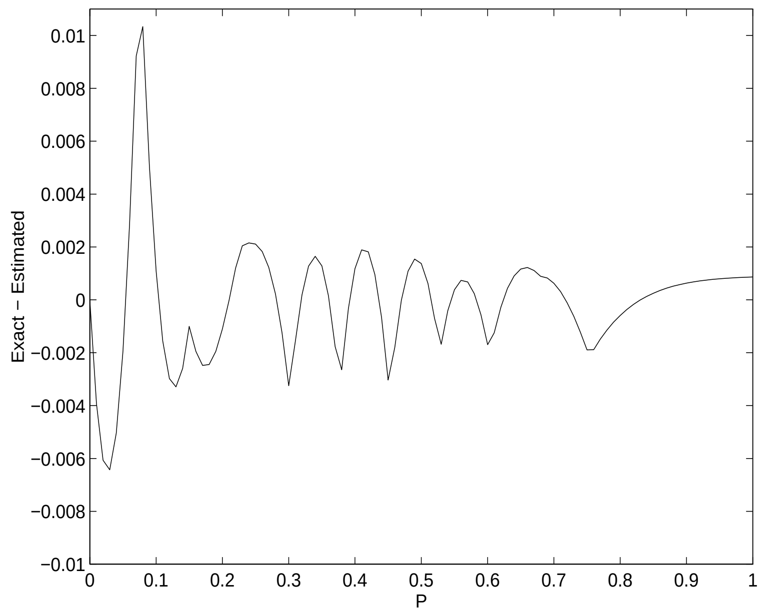

Figure 2: The difference between $a(P) = 0.9(1 - \exp(-10P^2))$ and the linear spline estimate $a_M(P)$.

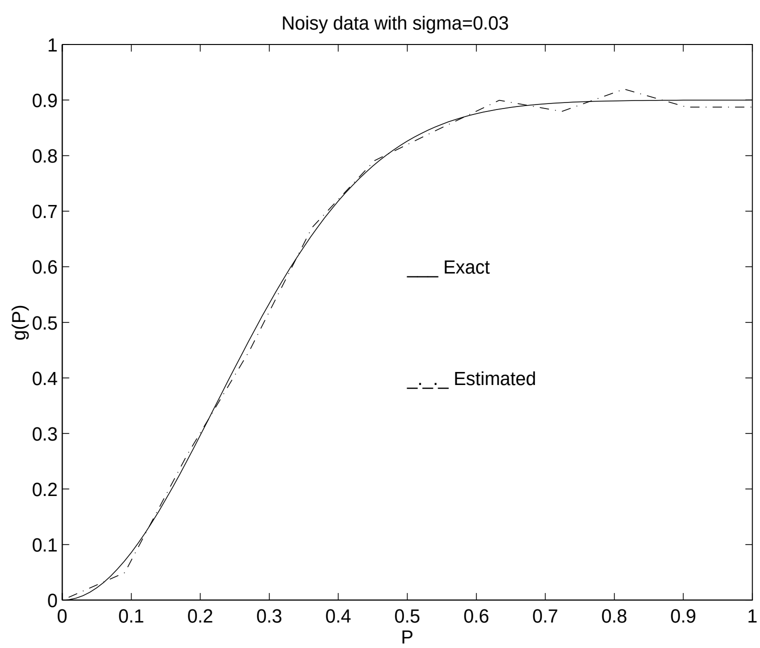

Figure 3: The function $a(P) = 0.9(1 - \exp(-10P^2))$ and the linear spline estimate $a_M(P)$.

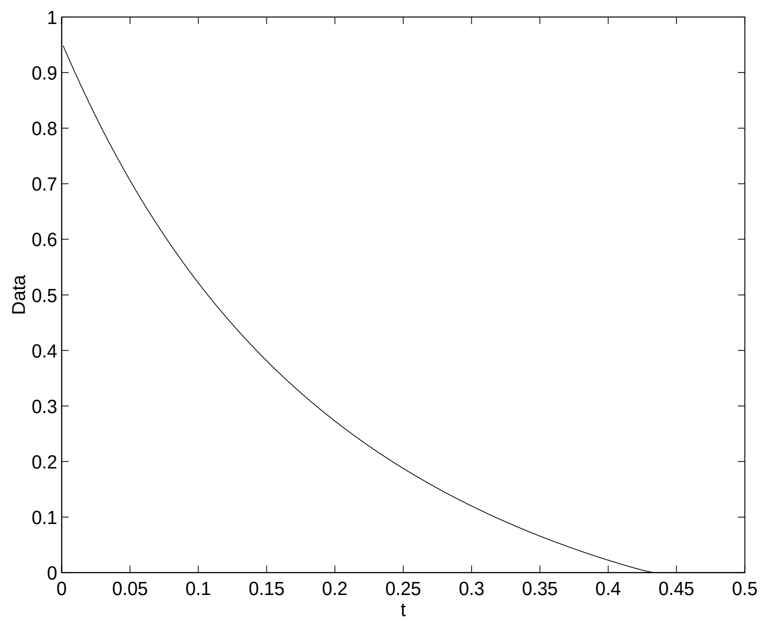

Figure 4: The computationally generated data with $a(P) = 0.7\frac{P}{0.05+P}$.

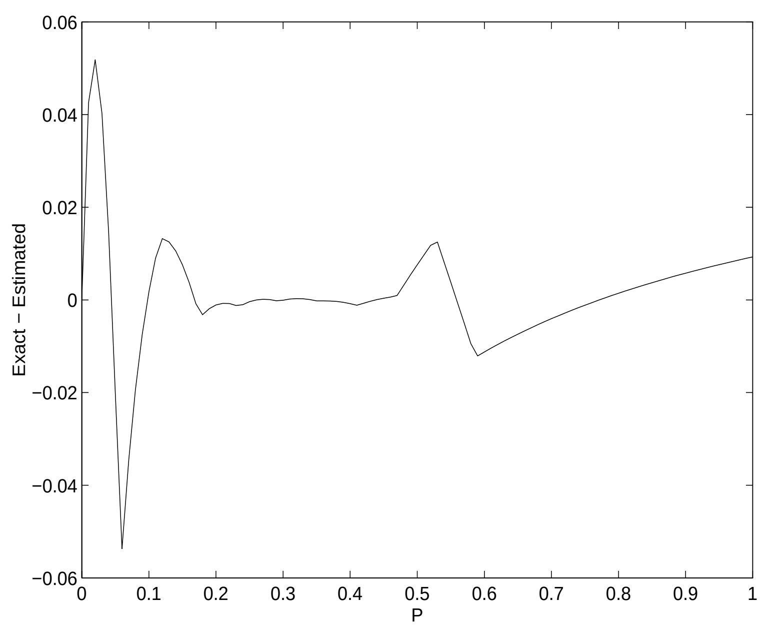

Figure 5: The difference between $a(P) = 0.7\frac{P}{0.05+P}$ and the linear spline estimate $a_M(P)$.

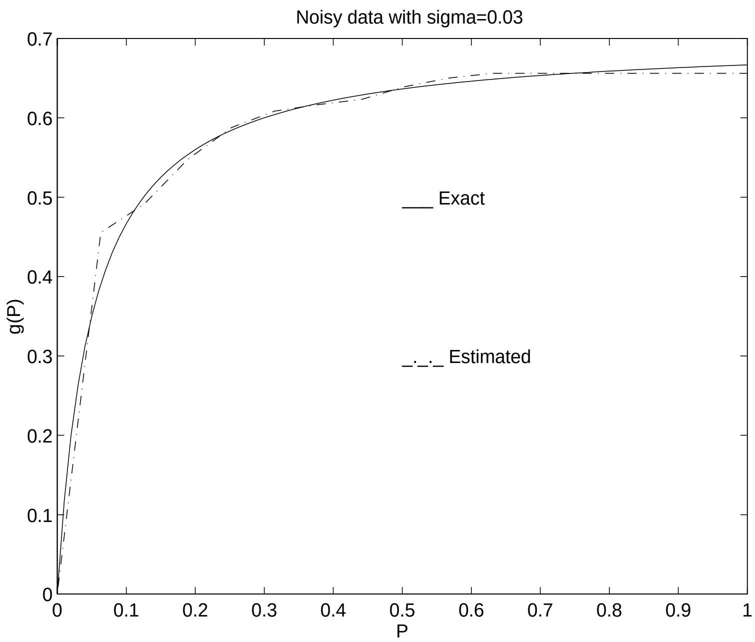

Figure 6: The function $a(P) = 0.7\frac{P}{0.05+P}$ and the linear spline estimate $a_M(P)$.

In (2.2) we used a mixed explicit-implicit approximation for the reaction function $uF(u)$. Our numerical experience indicates that this type of discretization provides a more accurate approximation near the extinction time of the population (the point where $\frac{1}{a(P)}$ has a singularity) than an explicit discretization. To obtain a similar accuracy using an explicit approximation for $uF(u)$ a smaller Δt was required resulting in more intensive computations. Our future efforts will focus on the development of a time adaptive finite difference scheme with an explicit approximation for the reaction term. We believe this will result in an efficient method that will not be computationally intensive since the adaptation of the time step size Δt will most likely play a major role only near the extinction time.

References

Ackleh, A.S., and L. Ke (1999). "Existence-Uniqueness and Long Time Behavior for a Class of Nonlocal Nonlinear Parabolic Evolution Equations", *Department of Mathematics Technical Report TR-99-03, University of Southwestern Louisiana, Lafayette, LA.*

Ackleh, A.S., R.R. Ferdinand, and S. Reich (1998). "Numerical Studies of Parameter Estimation Techniques for Nonlinear Evolution Equations", *Kybernetika*, **6**, pp. 693-712.

Ackleh, A.S., and S. Reich (1998). "Parameter Estimation in Nonlinear Evolution Equations", *Numerical Functional Analysis and Optimization*, **19**, pp. 933-947.

Banks, H.T., and K. Kunisch (1989). *Estimation Techniques for Distributed Parameter Systems,* Birkhäuser, Boston.

Banks, H.T., S. Reich, and I.G. Rosen (1990). "An Approximation Theory for the Identification of Nonlinear Distributed Parameter Systems", *SIAM Journal on Control and Optimization*, **28**, pp. 552-569.

Banks, H.T., S. Reich and I.G. Rosen (1991). "Galerkin Approximation for Inverse Problems for Nonautonomous Nonlinear Distributed Systems", *Applied Mathematics and Optimization*, **24**, pp. 233-256.

Bear, J. (1972). *Dynamics of Fluids in Porous Media,* Elsevier, New York.

M. Chipot, M., and B. Lovat (1999). "Existence and Uniqueness Results for a Class of Nonlocal Elliptic and Parabolic Problems", *manuscript obtained from internet: http://www.math.unizh.ch/~chipot/Quenching.ps.*

Freeze, R.A., and J. Cherry (1979). *Groundwater,* Prentice-Hall, Englewodd Cliffs, N.J.

Pao, C.V. (1992). *Nonlinear Parabolic and Elliptic Equations,* Plenum Press, New York.

Schultz, M.H. (1973). *Spline Analysis*, Prentice-Hall, Englewood Cliffs, N.J.