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PARAMETER ESTIMATION IN NONLINEAR COUPLED ADVECTION-DIFFUSION EQUATION

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Abstract

In this paper a coupled system of two nonlinear advection-diffusion equations is presented. Such systems of equations have been used in mathematical literature to describe the dynamics of contaminant present in groundwater flowing through cracks in a porous rock matrix and getting absorbed into it. An inverse method procedure that approximates infinite-dimensional model parameters is described and convergence results for the parameter approximants are proved. This is finally followed by a computational experiment to compare theoretical and numerical results to verify accuracy of the mathematical analysis presented.

Keywords: advection, coupled, diffusion, infinite-dimensional, parameter estimation

MSC: 65M06, 65M32, 65N06, 65N21

1. Introduction

A nonlinear coupled system of advection-diffusion PDEs that describes the dynamics of contaminant concentration in groundwater as it flows through cracks in a rocky, porous medium is presented below.

$$\begin{cases} u_t + [a(u)]_z = [b(u, u_z)]_z - \lambda u + \beta v_x(t, 0, z) \\ v_t = [e(v, v_x)]_x - \lambda v, \end{cases} \tag{1}$$

with initial and boundary conditions

$$\begin{cases} u(0, z) = \alpha(z), \quad u(t, 0) = \gamma(t), \quad u(t, z_{\max}) = 0 \\ v(0, x, z) = \eta(x, z), \quad v(t, 0, z) = \rho\, u(t, z), \quad v(t, x_{\max}, z) = 0. \end{cases} \tag{2}$$

The schematic diagram below illustrates the above phenomenon:

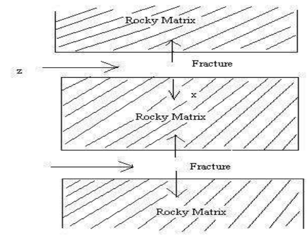

Figure 1: Schematic Diagram of Porous Fractured Rock

In the above model, the parameters are described as follows:

- $z \in \Omega = [0, z_{\max}]$: Distance along fracture
- $x \in \Lambda = [0, x_{\max}]$: Perpendicular distance into rock matrix
- $t \in \Gamma = [0, T_{\max}]$: Time
- $u(t, z)$: Contaminant concentration in liquid flowing through fracture in porous rock matrix at (t, z)
- $v(t, x, z)$: Contaminant concentration in liquid diffusing into rock matrix while flowing through fracture at (t, x, z)
- $a(u)$: Speed at which contaminant moves forward in liquid flowing through fracture
- $b(u, u_z)$: Rate at which contaminant diffuses in liquid flowing through fracture
- λ: Rate at which contaminant (radioactive) decays in time
- β: Rate at which contaminant in liquid moving in fracture gets absorbed into rocky matrix
- $e(v, v_x)$: Rate at which contaminant diffuses into rocky matrix
- $\alpha(z)$: Initial contaminant concentration in fracture
- $\gamma(t)$: Contaminant concentration in fracture at $x = 0$
- $\eta(x, z)$: Initial contaminant concentration in rocky matrix
- ρ: Fraction of contaminant diffusing into rocky matrix at $x = 0$

One may note that the generally nonlinear nature of the model parameters a, b and e indicates that the groundwater and rock matrix may not necessarily be homogeneous in their chemical compositions. This was one of the major reasons for studying this model, since in Sudicky and Frind (1982), these parameters are linear, indicating total homogeneity in the composition of the rock and water mediums. For a more detailed and exhaustive description of the physical phenomenon described by this model and definitions of the constants λ, β and ρ, the reader may refer to Sudicky and Frind (1982).

A forward Eüler finite difference method is used by the author in Ferdinand (2007) to obtain a numerical solution of model Eq.(1-2). This method will be described briefly, a little later in this manuscript. The goal of this paper, however, is to estimate infinite-dimensional parameters in the model using an inverse method procedure. This infinite-dimensional parameter estimation problem can be formally stated as follows:

Problem: Given observed model solution data

$$\begin{cases} \Pi_i = \int_0^{z_{\max}} u\left(t_i, z\right) \ dz \\ \\ \Theta_i = \int_0^{z_{\max}} \int_0^{x_{\max}} v\left(t_i, x, z\right) \ dx \ dz, \end{cases}$$

$i = 0, \cdots, X$, find an infinite-dimensional parameter vector $q = (a, b, e, \alpha, \gamma, \eta)$ so that the least-squares cost functional $J(q)$ is minimized over the infinite-dimensional parameter space Q, where

$$J(q) = \sum_{i=0}^{X} \left(\left| \int_0^{z_{\max}} u\left(t_i, z, q\right) \ dz - \Pi_i \right|^2 + \left| \int_0^{z_{\max}} \int_0^{x_{\max}} v\left(t_i, x, z, q\right) \ dx \ dz - \Theta_i \right|^2 \right) \tag{3}$$

and $(u(t, z, q), v(t, x, z, q))$ represents the parameter dependent solution of Eqs.(1-2).

To solve the above problem, one proceeds in this paper as follows. In the next section, an inverse method procedure is described which numerically approximates the infinite-dimensional parameter set q. Convergence results for these parameter approximants are proved while a numerical example illustrating the accuracy of these theoretical results is presented in section 3. Some concluding remarks are reported in section 4 while section 5 contains the reference information.

2. Inverse Method

To begin this section, the space D is defined as

$$D = C[0,\infty) \times C([0,\infty) \times (-\infty,\infty)) \times C([0,\infty) \times (-\infty,\infty)) \times C(\Omega) \times C(\Gamma) \times C(\Lambda \times \Omega),$$

with Q being a compact subset of D. Further, the following conditions are also satisfied by elements of set $q \in Q$.

(B1) a Lipschitz in u

(B2) b Lipschitz in u, u_z

(B3) e Lipschitz in v, v_x

(B4) $\alpha \in C^1(\Omega)$

(B5) $\gamma \in C^1(\Gamma)$

(B6) $\eta \in C^1(\Lambda \times \Omega)$

Techniques similar to those used in Ackleh (1999) and Ferdinand (2004) are used to solve this inverse problem. This procedure is well established and involves two steps which follow.

Step I: Numerically approximate parameter dependent model solution $(u(t,z,q), v(t,x,z,q))$ of Eqs.(1-2) using the following finite difference method from Ferdinand (2007):
Let

$$\Delta t = \frac{T_{\max}}{Y}, \qquad \Delta x = \frac{x_{\max}}{N} \qquad \text{and} \qquad \Delta z = \frac{z_{\max}}{R},$$

be uniform mesh sizes used for discretizing the t, x and z axes, respectively. This leads to

$$t_k = k\ \Delta t, \qquad x_j = j\ \Delta x \qquad \text{and} \qquad z_l = l\ \Delta z,$$

for $k = 0, \cdots, Y$, $j = 0, \cdots, N$ and $l = 0, \cdots, R$ being the axes mesh points. Use notation such as $v_{j,l}^k$ to represent $v(t_k, x_j, z_l)$ and so on to arrive at the following numerical scheme which computes the parameter dependent solution $\left(u_l^k(q), v_{j,l}^k(q)\right)$:

$$\left\{\begin{array}{rcl}
u_l^{k+1}(q) & = & (1-\lambda\ \Delta t)\, u_l^k(q) + \mu_1 \left[a\left(u_l^k(q)\right) - a\left(u_{l+1}^k(q)\right)\right. \\
& & \left. +b\left(u_l^k(q), \dfrac{u_{l+1}^k(q) - u_l^k(q)}{\Delta z}\right) - b\left(u_{l-1}^k(q), \dfrac{u_l^k(q) - u_{l-1}^k(q)}{\Delta z}\right)\right] \\
& & +\beta\ \mu_2\ \left(v_{1,l}^k(q) - \rho\ u_l^k(q)\right) \text{ for } l = 1, \cdots, R-1 \\
v_{j,l}^{k+1}(q) & = & (1-\lambda\ \Delta t)\, v_{j,l}^k(q) + \mu_2 \left[e\left(v_{j,l}^k(q), \dfrac{v_{j+1,l}^k(q) - v_{j,l}^k(q)}{\Delta x}\right)\right. \\
& & \left. -\ e\left(v_{j-1,l}^k(q), \dfrac{v_{j,l}^k(q) - v_{j-1,l}^k(q)}{\Delta x}\right)\right] \\
& & \text{for } j = 1, \cdots, N-1 \text{ and } l = 0, \cdots, R,
\end{array}\right. \tag{4}$$

where

$$\mu_1 = \frac{\Delta t}{\Delta z} \qquad \text{and} \qquad \mu_2 = \frac{\Delta t}{\Delta x},$$

while initial and boundary conditions give

$$\left\{\begin{array}{l}
u_l^0(q) = \alpha_l, \quad u_0^k(q) = \gamma^k, \quad u_R^k(q) = 0 \\
v_{j,l}^0(q) = \eta_{j,l}, \quad v_{0,l}^k(q) = \rho\ u_l^k(q), \quad v_{N,l}^k(q) = 0.
\end{array}\right. \tag{5}$$

Use (B1)-(B6) (see Ferdinand (2007)) to get that the solution approximants $\left\{\left(u_l^k\left(q\right), v_{j,l}^k\left(q\right)\right)\right\}$ obtained from Eqs.(4-5) above, converge to a unique parameter dependent solution, $\left(u\left(q\right), v\left(q\right)\right)$ of Eqs.(1-2) as $\Delta t,\ \Delta x,\ \Delta z \to 0$. In fact, one can extend these approximants to a family of functions as follows:

$$\left(U_{\Delta t,\Delta z}\left(t,z,q\right), V_{\Delta t,\Delta x,\Delta z}\left(t,x,z,q\right)\right) = \left(\left\{u_l^k\left(q\right)\right\}, \left\{v_{j,l}^k\left(q\right)\right\}\right),$$

when

$$t \in \left[t_{k-1}, t_k\right), \qquad x \in \left[x_{j-1}, x_j\right), \qquad z \in \left[z_{l-1}, z_l\right),$$

for

$$k = 1, \cdots, Y, \qquad j = 1, \cdots N, \qquad l = 1, \cdots, R.$$

This leads to the following computational form for J:

$$\begin{aligned} J_{\Delta t,\Delta x,\Delta z}\left(q\right) &= \sum_{i=0}^{X}\left(\left|\int_0^{z_{\max}} U_{\Delta t,\Delta z}\left(t_i,z,q\right)\ dz - \Pi_i\right|^2 \right. \\ &\left. + \left|\int_0^{z_{\max}}\int_0^{x_{\max}} V_{\Delta t,\Delta x,\Delta z}\left(t_i,x,z,q\right)\ dx\ dz - \Theta_i\right|^2\right) \end{aligned} \tag{6}$$

used in theorem 1 below.

Theorem 1. Using the convergence result $\left\|u_l^k - u\right\|_\infty \to 0$ and $\left\|v_{j,l}^k - v\right\|_\infty \to 0$ as $\Delta t, \Delta x, \Delta z \to 0$ in Ferdinand (2007), one arrives at

$$J_{\Delta t,\Delta x,\Delta z}\left(q\right) \to J\left(q\right)\ \text{ uniformly } \forall q \in Q. \tag{7}$$

Proof. Follows from convergence results for the solution approximants $\left(\left\{u_l^k\right\}, \left\{v_{j,l}^k\right\}\right)$ presented in detail in Ferdinand (2007).

Step II: Approximate the infinite-dimensional parameter space Q by a sequence $\left\{Q^M\right\}$ of finite-dimensional compact subsets of Q in the topology of D. An example of $\left\{Q^M\right\}$ is given in section 3. This further leads to the finite-dimensional computational form

$$\begin{aligned} J_{\Delta t,\Delta x,\Delta z}\left(q^M\right) &= \sum_{i=0}^{X}\left(\left|\int_0^{z_{\max}} U_{\Delta t,\Delta z}\left(t_i,z,q^M\right)\ dz - \Pi_i\right|^2 \right. \\ &\left. + \left|\int_0^{z_{\max}}\int_0^{x_{\max}} V_{\Delta t,\Delta x,\Delta z}\left(t_i,x,z,q^M\right)\ dx\ dz - \Theta_i\right|^2\right), \end{aligned} \tag{8}$$

$q^M \in Q^M$ being a finite-dimensional parameter vector, and one arrives at Theorem 2.

Theorem 2. For fixed values of $\Delta t, \Delta x$ and Δz

$$J_{\Delta t,\Delta x,\Delta z}\left(q^M\right) \to J_{\Delta t,\Delta x,\Delta z}\left(q\right)$$

as $q^M \to q$ in Q.

Proof. Let $\left(\left\{u_l^{k,M}\right\}, \left\{v_{j,l}^{k,M}\right\}\right)$ and $\left(\left\{u_l^{k}\right\}, \left\{v_{j,l}^{k}\right\}\right)$ represent the families of functions

$$\left(U_{\Delta t,\Delta z}\left(t,z,q^M\right), V_{\Delta t,\Delta x,\Delta z}\left(t,x,z,q^M\right)\right)$$

and

$$\left(U_{\Delta t,\Delta z}\left(t,z,q\right), V_{\Delta t,\Delta x,\Delta z}\left(t,x,z,q\right)\right),$$

respectively. Then let

$$\left(\bar{u}_l^{k,M}, \bar{v}_{j,l}^{k,M}\right) = \left(u_l^{k,M} - u_l^k, v_{j,l}^{k,M} - v_{j,l}^k\right)$$

for $k = 0, \cdots, Y$, $j = 0, \cdots, N$ and $l = 0, \cdots, R$. Boundary and initial conditions from Eq.(5) give

$$\left\{\begin{array}{lll} \bar{u}_l^{0,M} = \alpha_l^M - \alpha_l, & \bar{u}_0^{k,M} = \gamma^{k,M} - \gamma^k, & \bar{u}_R^{k,M} = 0 \\ \bar{v}_{j,l}^{0,M} = \eta_{j,l}^M - \eta_{j,l}, & \bar{v}_{0,l}^{k,M} = \rho\, \bar{u}_l^{k,M}, & \bar{v}_{N,l}^{k,M} = 0. \end{array}\right. \tag{9}$$

From the first of the two coupled equations in Eq.(4) get the operator forms

$$u_l^{k+1,M} = A_1 u_l^{k,M} \tag{10}$$

and

$$u_l^{k+1} = A_1 u_l^k \tag{11}$$

and subtract Eq.(11) from Eq.(10) to get

$$\begin{aligned} \left|\bar{u}_l^{k+1,M}\right| \leq\ & |1-\lambda\Delta t|\left|\bar{u}_l^{k,M}\right| \\ & +\mu_1\left|a^M\left(u_{l+1}^{k,M}\right) - a^M\left(u_l^{k,M}\right) - a\left(u_{l+1}^k\right) + a\left(u_l^k\right)\right| \\ & +\mu_1\left|b^M\left(u_l^{k,M}, \frac{u_{l+1}^{k,M} - u_l^{k,M}}{\Delta z}\right) - b\left(u_l^k, \frac{u_{l+1}^k - u_l^k}{\Delta z}\right)\right| \\ & +\mu_1\left|b^M\left(u_{l-1}^{k,M}, \frac{u_l^{k,M} - u_{l-1}^{k,M}}{\Delta z}\right) - b\left(u_{l-1}^k, \frac{u_l^k - u_{l-1}^k}{\Delta z}\right)\right| \\ & +\beta\,\mu_2\left|v_{1,l}^{k,M} - \rho\, u_l^{k,M} - v_{1,l}^k + \rho\, u_l^k\right|, \end{aligned} \tag{12}$$

which gives

$$\left|\bar{u}_l^{k+1,M}\right| \leq |1-\lambda\Delta t|\left|\bar{u}_l^{k,M}\right| + \mu_1\, I + \mu_1\, II + \mu_1\, III + \beta\,\mu_2\, IV. \tag{13}$$

Bounds need to be established for I, II, III and IV in Eq.(13). First let $\omega, \bar{\omega}, \omega_1 - \omega_9$ be positive constants. Then start with I, add and subtract terms to get

$$\begin{aligned} I \quad &\leq \quad \left| a^M \left(u_{l+1}^{k,M} \right) - a \left(u_{l+1}^{k,M} \right) + a \left(u_{l+1}^{k,M} \right) - a \left(u_{l+1}^{k} \right) \right| \\ &\quad + \left| a^M \left(u_{l}^{k,M} \right) - a \left(u_{l}^{k,M} \right) + a \left(u_{l}^{k,M} \right) - a \left(u_{l}^{k} \right) \right| . \end{aligned} \tag{14}$$

(B2) yields

$$I \leq \left| a^M \left(u_{l+1}^{k,M} \right) - a \left(u_{l+1}^{k,M} \right) \right| + \left| a^M \left(u_{l}^{k,M} \right) - a \left(u_{l}^{k,M} \right) \right| + \omega_1 \left| \bar{u}_{l+1}^{k,M} \right| + \omega_2 \left| \bar{u}_{l}^{k,M} \right| . \tag{15}$$

Add and subtract terms in II again to get

$$\begin{aligned} II \quad &\leq \quad \left| b^M \left(u_l^{k,M}, \frac{u_{l+1}^{k,M} - u_l^{k,M}}{\Delta z} \right) - b \left(u_l^{k,M}, \frac{u_{l+1}^{k,M} - u_l^{k,M}}{\Delta z} \right) \right| \\ &\quad + \left| b \left(u_l^{k,M}, \frac{u_{l+1}^{k,M} - u_l^{k,M}}{\Delta z} \right) - b \left(u_l^{k}, \frac{u_{l+1}^{k} - u_l^{k}}{\Delta z} \right) \right| . \end{aligned}$$

Similarly (B3) gives

$$II \leq \left| b^M \left(u_l^{k,M}, \frac{u_{l+1}^{k,M} - u_l^{k,M}}{\Delta z} \right) - b \left(u_l^{k,M}, \frac{u_{l+1}^{k,M} - u_l^{k,M}}{\Delta z} \right) \right| + \omega_3 \left(\left| \bar{u}_l^{k,M} \right| + \left| \bar{u}_{l+1}^{k,M} \right| \right) \tag{16}$$

and

$$III \leq \left| b^M \left(u_{l-1}^{k,M}, \frac{u_{l}^{k,M} - u_{l-1}^{k,M}}{\Delta z} \right) - b \left(u_{l-1}^{k,M}, \frac{u_{l}^{k,M} - u_{l-1}^{k,M}}{\Delta z} \right) \right| + \omega_4 \left(\left| \bar{u}_{l-1}^{k,M} \right| + \left| \bar{u}_{l}^{k,M} \right| \right) , \tag{17}$$

while

$$IV \leq \left| v_{1,l}^{k,M} - v_{1,l}^{k} \right| + \rho \ \left| u_l^{k,M} - u_l^{k} \right| = \left| \bar{v}_{1,l}^{k,M} \right| + \rho \ \left| \bar{u}_l^{k,M} \right| . \tag{18}$$

Now Eqs.(15-18) make Eq.(13) yield

$$\begin{aligned} \left| \bar{u}_l^{k+1,M} \right| \quad &\leq \quad \left| a^M \left(u_{l+1}^{k,M} \right) - a \left(u_{l+1}^{k,M} \right) \right| + \left| a^M \left(u_{l}^{k,M} \right) - a \left(u_{l}^{k,M} \right) \right| \\ &\quad + \left| b^M \left(u_l^{k,M}, \frac{u_{l+1}^{k,M} - u_l^{k,M}}{\Delta z} \right) - b \left(u_l^{k,M}, \frac{u_{l+1}^{k,M} - u_l^{k,M}}{\Delta z} \right) \right| \\ &\quad + \left| b^M \left(u_{l-1}^{k,M}, \frac{u_{l}^{k,M} - u_{l-1}^{k,M}}{\Delta z} \right) - b \left(u_{l-1}^{k,M}, \frac{u_{l}^{k,M} - u_{l-1}^{k,M}}{\Delta z} \right) \right| \\ &\quad + \omega_5 \left(\left| \bar{u}_l^{k,M} \right| + \left| \bar{u}_{l+1}^{k,M} \right| + \left| \bar{u}_{l-1}^{k,M} \right| + \left| \bar{v}_{1,l}^{k,M} \right| \right) . \end{aligned} \tag{19}$$

Next, proceed with the second of the two equations in Eq.(4) to arrive at

$$v_{j,l}^{k+1,M} = A_2 v_{j,l}^{k,M} \tag{20}$$

and

$$v_{j,l}^{k+1} = A_2 v_{j,l}^{k}. \tag{21}$$

Subtract Eq.(21) from Eq.(20) to get

$$\begin{aligned}\left|\bar{v}_{j,l}^{k+1,M}\right| &\leq |1-\lambda\Delta t|\left|\bar{v}_{j,l}^{k,M}\right| \\ &+\mu_2\left|e^M\left(v_{j,l}^{k,M},\frac{v_{j+1,l}^{k,M}-v_{j,l}^{k,M}}{\Delta x}\right)-e\left(v_{j,l}^{k},\frac{v_{j+1,l}^{k}-v_{j,l}^{k}}{\Delta x}\right)\right| \\ &+\mu_2\left|e^M\left(v_{j-1,l}^{k,M},\frac{v_{j,l}^{k,M}-v_{j-1,l}^{k,M}}{\Delta x}\right)-e\left(v_{j-1,l}^{k},\frac{v_{j,l}^{k}-v_{j-1,l}^{k}}{\Delta x}\right)\right|,\end{aligned} \tag{22}$$

which gives

$$\left|\bar{v}_{j,l}^{k+1,M}\right| \leq |1-\lambda\Delta t|\left|\bar{v}_{j,l}^{k,M}\right| + \mu_2\, V + \mu_2\, VI,$$

and bounds for V and VI are hence required. Start with V, use (B4) and follow techniques similar to those used in obtaining bounds for II and III to get

$$V \leq \left|e^M\left(v_{j,l}^{k,M},\frac{v_{j+1,l}^{k,M}-v_{j,l}^{k,M}}{\Delta x}\right)-e\left(v_{j,l}^{k,M},\frac{v_{j+1,l}^{k,M}-v_{j,l}^{k,M}}{\Delta x}\right)\right| + \omega_6\left(\left|\bar{v}_{j,l}^{k,M}\right|+\left|\bar{v}_{j+1,1}^{k,M}\right|\right) \tag{23}$$

and

$$VI \leq \left|e^M\left(v_{j-1,l}^{k,M},\frac{v_{j,l}^{k,M}-v_{j-1,l}^{k,M}}{\Delta x}\right)-e\left(v_{j-1,l}^{k,M},\frac{v_{j,l}^{k,M}-v_{j-1,l}^{k,M}}{\Delta x}\right)\right| + \omega_7\left(\left|\bar{v}_{j-1,l}^{k,M}\right|+\left|\bar{v}_{j,l}^{k,M}\right|\right). \tag{24}$$

Thus Eq.(22) yields

$$\begin{aligned}\left|\bar{v}_{j,l}^{k+1,M}\right| &\leq \left|e^M\left(v_{j,l}^{k,M},\frac{v_{j+1,l}^{k,M}-v_{j,l}^{k,M}}{\Delta x}\right)-e\left(v_{j,l}^{k,M},\frac{v_{j+1,l}^{k,M}-v_{j,l}^{k,M}}{\Delta x}\right)\right| \\ &+\left|e^M\left(v_{j-1,l}^{k,M},\frac{v_{j,l}^{k,M}-v_{j-1,l}^{k,M}}{\Delta x}\right)-e\left(v_{j-1,l}^{k,M},\frac{v_{j,l}^{k,M}-v_{j-1,l}^{k,M}}{\Delta x}\right)\right| \\ &+\omega_8\left(\left|\bar{v}_{j,l}^{k,M}\right|+\left|\bar{v}_{j+1,l}^{k,M}\right|+\left|\bar{v}_{j-1,l}^{k,M}\right|\right).\end{aligned} \tag{25}$$

Now pass the limit $q^M \to q$ in Q.

First, boundary and initial conditions in Eq.(9) yield

$$\left|\bar{u}_l^{0,M}\right|, \ \left|\bar{u}_0^{k,M}\right|, \ \left|\bar{u}_R^{k,M}\right|, \ \left|\bar{v}_{j,l}^{0,M}\right|, \ \left|\bar{v}_{N,l}^{k,M}\right| \to 0. \tag{26}$$

Next, Eq.(19) gives

$$\left|\bar{u}_l^{k+1,M}\right| \leq \omega_5 \left(\left|\bar{u}_l^{k,M}\right| + \left|\bar{u}_{l+1}^{k,M}\right| + \left|\bar{u}_{l-1}^{k,M}\right| + \left|\bar{v}_{1,l}^{k,M}\right|\right). \tag{27}$$

Further, Eq.(25) leads to

$$\left|\bar{v}_{j,l}^{k+1,M}\right| \leq \omega_8 \left(\left|\bar{v}_{j,l}^{k,M}\right| + \left|\bar{v}_{j+1,l}^{k,M}\right| + \left|\bar{v}_{j-1,l}^{k,M}\right|\right), \tag{28}$$

and finally

$$\left|v_{0,l}^{k+1,M}\right| \leq \rho\, \omega_5 \left(\left|\bar{u}_l^{k,M}\right| + \left|\bar{u}_{l+1}^{k,M}\right| + \left|\bar{u}_{l-1}^{k,M}\right| + \left|\bar{v}_{1,l}^{k,M}\right|\right). \tag{29}$$

Thus Eqs.(26-29) give

$$\begin{aligned} \left|\bar{u}_l^{k+1,M}\right| + \left|\bar{v}_{j,l}^{k+1,M}\right| \quad \leq \quad & \omega_9 \left(\left|\bar{u}_l^{k,M}\right| + \left|\bar{u}_{l+1}^{k,M}\right| + \left|\bar{u}_{l-1}^{k,M}\right| + \left|\bar{v}_{1,l}^{k,M}\right| \right. \\ & \left. + \left|\bar{v}_{j,l}^{k,M}\right| + \left|\bar{v}_{j+1,l}^{k,M}\right| + \left|\bar{v}_{j-1,l}^{k,M}\right|\right). \end{aligned} \tag{30}$$

Now define

$$\Upsilon^{k,M} = \max_{j=0,\cdots,N\ ;\ l=0,\cdots,R} \left(\left|\bar{u}_l^{k,M}\right| + \left|\bar{v}_{j,l}^{k,M}\right|\right).$$

This results in Eq.(30) giving

$$\Upsilon^{k+1,M} \leq \omega_9 \Upsilon^{k,M} \Rightarrow \Upsilon^{k,M} \leq \bar{\omega} \Upsilon^{0,M}.$$

Eq.(26) easily yields $\Upsilon^{0,M} \to 0$ which leads to $\Upsilon^{k,M} \to 0$. Hence, one gets that

$$\left(\bar{u}_l^{k,M}, \bar{v}_{j,l}^{k,M}\right) \to (0,0) \Rightarrow \left(u_l^{k,M}, v_{j,l}^{k,M}\right) \to \left(u_l^k, v_{j,l}^k\right),$$

thereby leading to $J_{\Delta t,\Delta x,\Delta z}\left(q^M\right) \to J_{\Delta t,\Delta x,\Delta z}\left(q\right)$ which concludes the proof of this theorem and leads to corollary 3 below.

Corollary 3. $J_{\Delta t,\Delta x,\Delta z}\left(q^M\right) \to J_{\Delta t,\Delta x,\Delta z}\left(q\right) \to J\left(q\right)$ when $\Delta t, \Delta x, \Delta z \to 0$ and $q^M \to q$ in Q as $M \to \infty$.

Proof. Follows from proofs of Theorems 1 and 2 above.

Corollary 3 above shows J to be a continuous functional over each of the compact subsets Q^M of Q in the sequence $\left\{Q^M\right\}$ and leads to J having a minimizer $\overline{q}^M \in Q^M$ over each Q^M. Using the abstract least-squares theory presented in Banks and Kunisch (1989), this sequence of minimizers $\left\{\overline{q}^M\right\}$ has a subsequence converging to a minimizer $\overline{\overline{q}} \in Q$ of $J(q)$ over set Q in the topology of D. Hence one arrives at the existence of a solution to the inverse problem stated earlier.

In the next and final section, a numerical example is presented to illustrate accuracy of the theoretical results proved in this section.

3. Numerical Experiment

To begin with, observed data is generated computationally. In order to accomplish this, parameters of the model equation Eqs.(1-2) are given the following known values:

- $x_{\max} = z_{\max} = 1.0,\ T_{\max} = 2.5 \times 10^{-2}$
- $\Delta x = \Delta z = 1.0 \times 10^{-1},\ \Delta t = 10^{-4}$
- $\lambda = \beta = \rho = 1.0$
- $a(u) = u^2,\ b(u, u_z) = (uu_z)^2,\ e(v, v_x) = (vv_x)^2$
- $\alpha(z) = (z-1)^2,\ \gamma(t) = e^{-t},\ \eta(x, z) = (x-1)^2(z-1)^2$

It would be worthwhile to mention that nonlinear a, b and e in the list above represent nonhomogeneity in the composition of liquid and contaminant. It should also be noted that these parameter values are chosen for the sole purpose of validating the theoretical results proved earlier and may not necessarily represent a real-life phonemenon in particular.

The parameter to be estimated numerically is the function a. The other unknown parameters $b, e, \alpha, \gamma, \eta$ can be approximated in a similar fashion. To accomplish this, the model equation Eqs.(1-2) is solved numerically to obtain the following data:

$$\left\{\begin{array}{l}\Pi_i = \displaystyle\int_0^1 u(t_i, z)\ dz \\[2ex] \Theta_i = \displaystyle\int_0^1 \int_0^1 v(t_i, x, z)\ dz\ dx,\end{array}\right.$$

where

$$t_i = 0.0005i, \qquad i = 0, \cdots, 50.$$

Now choose the infinite-dimensional parameter space Q for this experiment as the D-closure of the set

$$\left\{|a(u)| \le L, |a(u_1) - a(u_2)| \le L|u_1 - u_2|, \forall u_1, u_2 \in [0, \infty), a = L \text{ for } u \ge u_{\max}\right\}, \tag{31}$$

L and $u_{\max}$ being fixed constants. Hence, Q follows as a compact subset of D from the Arzèla-Ascoli theorem.

To implement **Step II**, Q is approximated numerically by a sequence $\left\{Q^M\right\}$ of finite-dimensional compact subsets in the topology of D. Each Q^M uses the set of linear splines $\left\{\psi_j^M\left(u; u_{\max}\right)\right\}_{j=0}^{M}$ on a uniform partition of $[0, u_{\max}]$ as its approximating elements. Thus, the unknown parameter $a\left(u\right)$ is approximated over each Q^M in the form of the interpolant

$$I^M\left(a\right) = \sum_{j=0}^{M} a\left[j\frac{u_{\max}}{M}\right]\ \psi_j^M\left(u; u_{\max}\right), \qquad u \in [0, \infty) \tag{32}$$

with a extended to a continuous function on $[0, \infty)$ by letting $\psi_j^M\left(u; u_{\max}\right) = \psi_j^M\left(u_{\max}; u_{\max}\right)$ when $u \geq u_{\max}$, for $j = 0, \cdots, M$.

The Peano kernel theorem in Schultz (1973) leads to $\lim_{M\to\infty} I^M\left(a\right) = a$. Hence, if $a^M \in Q^M$ is represented as

$$a^M\left(u\right) = \sum_{j=0}^{M} \zeta_j^M \psi_j^M\left(u; u_{\max}\right),$$

then the numerical parameter estimation problem involves the identification of $(M+2)$ unknown constants $\zeta_j : j = 0, \cdots, M$ and $u_{\max}$ so that $J_{\Delta t, \Delta x, \Delta z}\left(a^M\right)$ is minimized. This is performed computationally using Eq.(4) and the *FORTRAN* subroutine *LMDIF1*, obtained from *NETLIB*, that implements the *Levenberg-Marquardt* algorithm with all integrals computed numerically using Simpson's rule of integration. Next,

$$\zeta_j^M = 0.5 : j = 0, \cdots, M \qquad \text{and} \qquad u_{\max} = 1$$

are taken as initial guesses and the following results are obtained.

(i) Figure 2 below shows a comparison between exact and estimated function $a\left(u\right) = u^2$ when $M = 9$. Exact function here is given by the straight line graph while the estimated function is given by the dots. $u_{\max}$ is estimated here as 0.98 and the value of $J_{\Delta t, \Delta x, \Delta z}\left(a^9\right)$ at the end of the experiment is of the order of 10^{-5}. This estimation took about 2 hours of computing time on a UNIX machine.

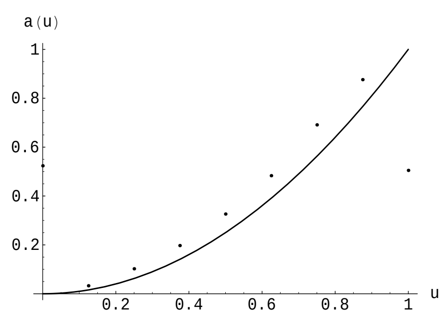

Figure 2: Exact Function - Solid Line; Estimated Function - Dots

(ii) Figure 3 below shows the same for $M = 11$. Estimation of $u_{\max}$ was once again 0.98 and $J_{\Delta t,\Delta x,\Delta z}(a^{11})$ at the end of the experiment came out to be of the order of 10^{-6}. Computing time was about 2 hours on a UNIX machine.

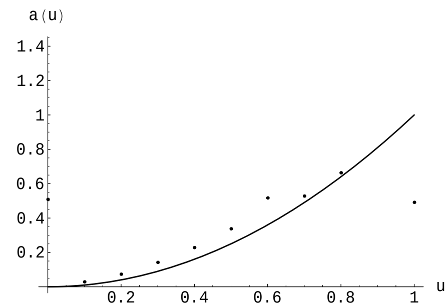

Figure 3: Exact Function - Solid Line; Estimated Function - Dots

4. Closing Comments

It would be worthwhile to mention that the computational estimation was performed in the *FORTRAN* programming language executed on a *UNIX* machine at East Central University in Ada, OK, USA. This facility is an SCO UNIX 5.0.5 machine, consisting of two 550 MHz Xeon processors in parallel. Both the above graphs were plotted using *MATHEMATICA* which proved to be extremely efficient for this purpose.

Further, it may also be noted by looking at Figures 2 and 3, that the numerical estimation of $a(u) = u^2$ is more accurate towards the interior of $[0, u_{\max}]$. This is owing to a much higher concentration of observed data present in the interior as opposed to the boundaries of this interval. Hence one concludes this section and also this paper by stating that numerical results obtained herein illustrate the accuracy of the theoretical results proved in section 2.

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