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Using Empirical Eigenfunctions and Galerkin Method to Two-Phase Transport Models

Abdollah Shidfar, Masoumeh Mohammadi
Department of Mathematics, Iran University of Science and Technology, Narmak, Tehran 16844, Iran

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In this article, we consider a nonlinear partial differential system describing two-phase transports and try to recover the source term and the nonlinear diffusion term when the state variable is known at different profile times. To this end, we use a POD-Galerkin procedure in which the proper orthogonal decomposition technique is applied to the ensemble of solutions to derive empirical eigenfunctions. These empirical eigenfunctions are then used as basis functions within a Galerkin method to transform the partial differential equation into a set of ordinary differential equations. Finally, the validation of the used method has been evaluated by some numerical examples. © 2006 Wiley Periodicals, Inc. Numer Methods Partial Differential Eq 23: 456–474, 2007

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1. INTRODUCTION

The two-phase modeling has been increasingly used in a variety of applications including the petroleum industry, chromatography, aggregated/structured soils, stratified soils, solute transport and multiphase applications. These models often lead to a system of parabolic partial differential equations (PDE). Since, a finite number of dominant modes of parabolic PDE systems practically determines the system dynamics [1], the dynamic behavior of such systems can be represented by finite-dimensional systems. For this reason, the Galerkin method has been used extensively to construct numerical solutions to parabolic PDEs [2]. The idea is to replace the given dynamics by an associated dynamics in which the PDE system is reduced to a set of ordinary differential equations that accurately describe the dominant dynamics of the PDE system. However, when the under consideration parabolic PDE system includes nonlinear spatial differential operator, Galerkin method cannot be directly employed. This obstacle is caused by difficulty in solving the eigenvalue problem of nonlinear spatial differential operators. Indeed, one cannot expect a predetermined basis to capture all the system dynamics. An appropriate approach to generate the necessary basis is applying the proper orthogonal decomposition technique to an ensemble of the PDE system solutions to derive empirical eigenfunctions of the system. The empirical eigenfunctions are then

Correspondence to: Abdollah Shidfar, Department of Mathematics, Iran University of Science and Technology, Narmak, Tehran 16844, Iran (email: shidfar@iust.ac.ir)

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used as basis functions in Galerkin method. This procedure which combines Galerkin method with such empirical eigenfunctions is called the proper orthogonal decomposition (POD)-Galerkin method or the Karhunen-Loève Galerkin procedure.

This article is organized as follows. In section 2, we present a model describing many dual transfers. The model reduction and POD-Galerkin procedure are given in section 3. This section also contains the theoretical aspects of POD method. In section 4 we employ the model reduction technique and apply the POD-Galerkin procedure to provide the means to identify the model unknown parameters from observed data using empirical eigenfunctions. The long-term behavior of the system is also discussed there. Section 5 contains some numerical examples that estimate the unknown parameters from computationally generated data and proceeds to method validation. Finally, throughout section 6 we conclude the article with a summary.

2. GOVERNING SYSTEM OF EQUATIONS

According to proposed models for solute transport in a dual porosity media such as [3], we consider two phases to describe the transport processes that can be used also for living systems [4]. That is, we will have two different but dependent equations: a diffusion-convection-reaction equation with nonlinear diffusion coefficient in mobile phase and a first-order reaction in immobile phase.

Mobile phase:

$$\varepsilon\frac{\partial C}{\partial t}+\frac{\partial}{\partial t}(\rho_s C_s)=\varepsilon\frac{\partial}{\partial x}\left(D(C)\frac{\partial C}{\partial x}\right)-\varepsilon\frac{\partial}{\partial x}(vC)+(R_{gf}-R_{df}). \tag{2.1}$$

Immobile phase:

$$\frac{\partial}{\partial t}(\rho_s C_s)=(R_c-R_r)+(R_{gs}-R_{ds}), \tag{2.2}$$

for time $t\in(0,\infty)$ and position x in some domain $\Omega\subset\mathbf{R}$, where x is a vertical coordinate directed downward.

In the equations above, C, C_s are, respectively, concentrations in the mobile and immobile phases; ε is the media porosity; $D(C)$ is diffusion coefficient; v is velocity; ρ_s is the media bulk density; ρ_b is solute density; $R_{gf}=k_{gf}\varepsilon C$, $R_{df}=-k_{df}\varepsilon C$ are, respectively, rate of growth (production) and decay of freely suspended particles (cells); $R_{gs}=k_{gs}\rho_b C_s$, $R_{ds}=-k_{ds}\rho_b C_s$ are, respectively, rate of growth and decay of sessile particles (cells); $R_r=k_r\rho_b C_s$, $R_c=k_c\varepsilon C$ are, respectively, rate of release of captured and capture of suspended particles (cells), where positive coefficients k with different subscripts indicate special coefficients; for example, k_{gf} is the specific growth rate of free particles (cells).

Set $\Omega=(-1,1)$; The initial and boundary conditions can be written as:

$$\begin{aligned}\frac{\partial}{\partial x}C(-1,t)&=0, \qquad t>0,\\ C(1,t)&=\gamma(t), \qquad t>0,\\ C(x,0)&=C^0(x), \qquad x\in\Omega,\\ C_s(x,0)&=C_s^0(x), \qquad x\in\Omega.\end{aligned} \tag{2.3}$$

However, as it will be observed soon, since the unknown parameters finding method is based on a predetermined ensemble of solutions, our approach allows for the flexibility in boundary and

initial conditions. That is they may be choose different from which we have introduced here to encompass real situations.

Our aim is to estimate the mobile concentration C in the domain for $t > 0$ as well as the initial immobile concentration C_s^0 and the nonlinear diffusion coefficient $D(C)$ by measuring the mobile concentration at many different times, where $C^0(x)$ and $\gamma(t)$ are some known functions.

In order to meet these objectives, our approach is as follows. We have at once from (2.2) that

$$C_s = e^{\alpha_1 t} C_s^0(x) + \alpha_2 \int_0^t e^{\alpha_1 (t-s)} C(x,s) ds, \tag{2.4}$$

where $\alpha_1 = (\rho_b/\rho_s)(-k_r + k_{gs} + k_{ds})$ and $\alpha_2 = (k_c \varepsilon/\rho_s)$.

By substitution (2.4) into (2.1), we obtain

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x}\left(D(C)\frac{\partial C}{\partial x}\right) - v\frac{\partial C}{\partial x} + \beta_1\left(e^{\alpha_1 t} C_s^0(x) + \alpha_2 \int_0^t e^{\alpha_1 (t-s)} C(x,s) ds\right) + \beta_2 C, \tag{2.5}$$

in which $\beta_1 = -(\rho_s \alpha_1/\varepsilon), \beta_2 = k_{gf} + k_{df} - (\rho_s \alpha_2/\varepsilon)$.

Here, for the sake of brevity consider the following changes:

$$u(x,t) = \frac{1}{\beta_1} e^{-\alpha_1 t} C(x,t),$$

$$u_0(x) = \frac{1}{\beta_1} C^0(x),$$

$$f(x) = C_s^0(x),$$

and let $\gamma(t) = k e^{\alpha_1 t}$, where k is a very small value.

Applying this notation to (2.5) and (2.3), our problem for $x \in \Omega$ and $t > 0$ is transformed in

$$\begin{aligned}
&\frac{\partial u}{\partial t} + \mathcal{A}u = f(x) + \beta_1 \alpha_2 \int_0^t u(s) ds + (\beta_2 - \alpha_1) u, \\
&\frac{\partial}{\partial x} u(-1,t) = 0, \\
&u(1,t) = \frac{k}{\beta_1}, \\
&u(x,0) = u_0(x),
\end{aligned} \tag{2.6}$$

where $\mathcal{A}$ is a nonlinear spatial differential operator of the form

$$\mathcal{A} = -\frac{\partial}{\partial x}\left(D(C)\frac{\partial}{\partial x}\right) + v\frac{\partial}{\partial x}.$$

Since the constant k/β_1 is negligible because k is small particularly in respect of β_1, considering $u(1,t) = 0$ seems an equivalent but simpler condition that we prefer. We proceed to find unknown parameters in section 4 using the method introduced in the next section.

3. MODEL REDUCTION BY POD-GALERKIN PROCEDURE

In this section, we present a method for developing a reduced order nonlinear model of PDE systems in the form of (2.6). To be computationally feasible, model reduction is an attractive means to arrive at simplified dynamical descriptions of the behavior of a complicated nonlinear partial

differential equations system. Reduction approach is based on building a low-order nonlinear model that can be described by a number of ordinary differential equations. The simplest way to this end is to assume that the dominant dynamics of the underlying system can be represented by a finite linear combination of basis functions.

From this point of view, the Galerkin method, which has been widely used to approximate and reduce a system of PDEs to a set of ODEs, is a model reduction means. In general we can choose an appropriate basis functions, $\{\psi_k(x)\}_{k=1}^{\infty}$ and in consequence, reach to a good approximation of the state variable u in (2.6) by spatial expansion in basis functions

$$u(x,t) = \sum_{k=1}^{\infty} \psi_k(x) a_k(t),$$

where the coefficients $a_k(t)$, are to be determined. The main idea in the Galerkin method is to construct basis functions that will have the lowest number of basis coefficients and yet reproduce the system dynamics accurately. The number of time-varying coefficients $a_k(t)$ involved in representing the state variable u could be reduced if the basis functions were similar in form to the actual solution of the system. In this case, we can employ a finite number of basis functions referred to as dominant or slow modes rather than an infinite number to approximate u:

$$u(x,t) \simeq \sum_{k=1}^{N} \psi_k(x) a_k(t).$$

One approach to meet this end is to use the eigenfunctions of spatial differential operator $\mathcal{A}$ in (2.6), as analytical basis functions (which is sometimes referred to as the eigenfunctions method [5]). But when the spatial differential operator poses a nonlinear form as in our model, the corresponding eigenvalue problem can not be solved analytically. Furthermore, in our model not only the operator $\mathcal{A}$ has a nonlinear term but this term has an unknown parameter. In contrast, there is a good understanding of the system behavior. Under these circumstances, using the POD technique, which only needs an ensemble of system solutions to obtain approximating functions that capture all the system dynamics, seems a very appropriate approach. This procedure which combines the Galerkin method with empirical eigenfunctions extracted by employing POD technique is called the POD-Galerkin procedure (also known as the Karhunen-Loève Galerkin procedure).

In summary, this procedure requires three steps in model reduction as follows. The first step is construction of a representative ensemble from an ensemble of solutions of the PDE system for different time profiles; The second step is to process the ensemble by the POD method and derive empirical eigenfunctions. Construction of the reduced order model through Galerkin method with empirical eigenfunctions is the last step. For more details and error analysis, see [6].

Additionally, as it will be mentioned soon, since POD technique constructs an orthonormal set of functions, it is possible to find an approximation of the unknown function $f(x)$ in terms of a linear combination of the orthonormal set of empirical eigenfunctions, which provides a very useful means to deal with the inverse problem.

A. Theory

The POD method is based on statistical analysis of data and has been used in a variety of fields such as fluid dynamics, image processing, pattern recognition, signal analysis, model reduction and control in chemical engineering. This method has appeared in the literature under a large number of different names depending on the area of application, including: principal component

analysis, Hotelling transform, Karhunen-Loève decomposition, empirical eigenfunctions, empirical orthogonal eigenfunctions, empirical mode decomposition, factor analysis, and total least squares. This method was first suggested by Lumley [7] as a tool for the extraction of coherent structures in turbulent flows and recently, due to its expanded applications has received essential attention. POD used to construct nonlinear low-order approximation of parabolic PDEs and nonlinear controllers was initially proposed in [8]. For utilizing this technique in the context of optimization of the transport-reaction process, the interested reader is referred to [9, 10]. Here, we briefly review this method. Further information can be found in [11–14].

To construct empirical eigenfunctions using POD method, suppose we have an ensemble of scalar functions $u_t(x) \in \mathcal{H}$ called snapshots, which denote the empirical solutions of the PDE system (2.6) at N different times, obtained either from experimental observations or from numerical simulations. Let $\mathcal{H}$ be a Hilbert space consist of smooth functions on spatial domain Ω, for instance, $\mathcal{H} = L^2(\Omega)$. For simplicity assume that the time intervals between two successive snapshots are equal.

Although in [15], you can find an overview of the general method of POD and Galerkin projection in the context of an abstract Hilbert space, we assume the standard L^2 inner product and the norm as follows:

$$(\psi_1, \psi_2) = \int_\Omega \psi_1(x)\psi_2(x)dx, \qquad \|\psi_1\|_2 = (\psi_1, \psi_1)^{1/2},$$

where ψ_1, ψ_2 are two elements of $\mathcal{H}$. Throughout this article we use this assumption unless we mention.

Also we denote the temporal averaging operation by $\langle\cdot\rangle$. By subtracting out the ensemble average of snapshots $\langle\bar{u}(x)\rangle = \frac{1}{N}\sum_{t=1}^{N} u_t(x)$, from the snapshots, i.e., $v_t(x) = u_t(x) - \langle\bar{u}(x)\rangle$, we focus on the deviations from the mean. We would like to find $\varphi(x)$ so that this basis function describes the ensemble of N temporal deviations $v_t(x)$ better than any other linear basis. Mathematically, the minimization of the difference between these deviations (and consequently the data snapshots) and their representative basis is equivalent to maximizing the ensemble average of the inner product between φ and v_t [16]:

$$\text{Maximize}\frac{\langle(\varphi, v_t)^2\rangle}{(\varphi, \varphi)}, \qquad s.t.\ (\varphi, \varphi) = 1.$$

The normalization constraint $\|\varphi\|_2 = 1$ is imposed to ensure that the function $\varphi(x)$, computed as a solution to the above maximization problem, is unique. The Lagrangian functional corresponding to this constrained optimization problem is

$$\bar{L} = \langle(\varphi, v_t)^2\rangle - \lambda((\varphi, \varphi) - 1),$$

where λ is a Lagrange multiplier. Since we can write

$$\langle(\varphi, v_t)^2\rangle = \frac{1}{N}\sum_{t=1}^{N}(\varphi(x), v_t(x))^2 = \int_\Omega\int_\Omega \frac{1}{N}\sum_{t=1}^{N}\varphi(x)\varphi(x')v_t(x')dx'v_t(x)dx,$$

after using the calculus of variations and some amount of algebra, the optimality condition takes the form

$$\int_\Omega \langle v_t(x)v_t(x')\rangle\varphi(x')dx' = \lambda\varphi(x), \qquad (\varphi, \varphi) = 1.$$

If the usual ergodicity hypothesis is invoked, the two-point correlation function is given by

$$K(x,x') = \langle v_t(x)v_t(x')\rangle = \frac{1}{N}\sum_{t=1}^{N} v_t(x)v_t(x'),$$

and consequently the problem of extracting the best basis function or in other words obtaining the empirical eigenfunction reduces to the following eigenvalue problem of the integral equation

$$\int_{\Omega} K(x,x')\varphi(x')dx' = \lambda\varphi(x). \tag{3.1}$$

Now we have to solve a high-order eigenvalue problem. To meet this problem, Sirovich has developed the method of snapshots that reduces the order of the solution to that of an eigenvalue problem of size equal to the number of snapshots [13]. In this method it is assumed that the basis function $\varphi(x)$ is a linear combination of the snapshots, i.e., $\varphi(x) = \sum_{t=1}^{N} c_t v_t(x)$. Substituting this form into (3.1), our problem reduces to solving the following matrix eigenvalue problem

$$\int_{\Omega} \frac{1}{N}\sum_{t=1}^{N} v_t(x)v_t(x')\sum_{t=1}^{N} c_t v_t(x)dx' = \lambda\sum_{t=1}^{N} c_t v_t(x).$$

Defining

$$a_{ij} = \frac{1}{N}\int_{\Omega} v_i(x)v_j(x)dx,$$

the above eigenvalue problem with setting $A = (a_{ij})$ takes the form

$$Ac = \lambda c.$$

The matrix A is called the ensemble averaged covariance matrix.

As soon as obtaining the eigenvectors $c^{(k)} = \left[c_1^{(k)} \cdots c_N^{(k)}\right], k = 1,2,\ldots,N$, the empirical eigenfunctions are computed as follows:

$$\varphi_k(x) = \sum_{t=1}^{N} c_t^{(k)} v_t(x).$$

Each eigenvalue represents the contribution of the corresponding eigenfunction to the total energy [12]. Therefore, the eigenfunctions corresponding to the largest eigenvalues λ are the most important modes in characterizing the system.

Because A is a symmetric and positive semi-definite $N \times N$ matrix, its eigenvalues, $\lambda_k, k = 1,\ldots,N$ are real and non-negative. Furthermore, the kernel of the integral equation (3.1) is symmetric, and thus the corresponding sets of empirical eigenfunctions are orthonormal.

Although, in our approach we use the spatial eigenfunctions, in [17] there is a methodology for retrieving spatial and temporal eigenfunctions from an ensemble of data, using POD, and it can be considered that the efficiency of these two families of eigenfunctions can be different when used in model reduction projections.

4. APPLICATION TO GOVERNING EQUATIONS

In this section an inverse problem for the initial-boundary value problem introduced in section 2 is considered and solved. The under consideration inverse problem is the task of estimating three parameters of the model with governing Equations (2.1)–(2.3), namely concentration $C(x,t)$, nonlinear diffusion coefficient $D(C)$, and the initial concentration of sessile cells $C_s^0(x)$. Due to our attempt to develop a mathematical model to fit the observed data (or a predetermined one using a numerical method), our inverse problem is often called as a modeling problem. In general, inverse problems are difficult to solve. These problems have been discussed in the literature by many authors such as Canon [18], Beck [19], and Shidfar [20–22]. Here, to solve the inverse problem we use the POD-Galerkin method proposed in section 3, which provides fast and accurate solutions. Throughout section 2, we applied some calculus that in consequence, the inverse problem we discuss is the following:

Given observations $u_{t_i}(x) \in \mathcal{H}$ at times $0 < t_1 < t_2 < \cdots < t_N$, where $N \geq 1$ and u_0 is a known function in $\mathcal{H}$, find u, D, f verifying

$$\begin{aligned} \frac{\partial u}{\partial t} + \mathcal{A}u &= f(x) + \alpha \int_0^t u(s)ds - \beta u, \\ \frac{\partial}{\partial x}u(-1,t) &= 0, \\ u(1,t) &= 0, \\ u(x,0) &= u_0(x), \end{aligned} \tag{4.1}$$

subject to

$$\min \ \|u_{t_i}(x) - u(x,t_i)\|. \tag{4.2}$$

Recall that $\mathcal{A}$ is a nonlinear spatial differential operator of the form

$$\mathcal{A} = -\frac{\partial}{\partial x}\left(D(C)\frac{\partial}{\partial x}\right) + v\frac{\partial}{\partial x},$$

where α and β are some constants [see (2.6)].

The procedure employed to construct the POD modes in the previous section leads to the following.

Proposition 4.1. *Suppose $\mathcal{S}$ be a subset of $\mathcal{H}$ with empirical eigenfunctions extracted by POD method as basis. If u in the problem 4.1 belongs to $\mathcal{S}$, then the optimality condition 4.2 is satisfied.*

Therefore, since in our approach to solve the problem, we seek u in the space spanned by POD modes, we ignore the optimality condition 4.2.

A. The Long-term Behavior of the System

First, let us introduce a hypothesis on $\mathcal{A}$.

Hypothesis. An orthonormal sequence of basis functions $\psi_k(x) \in \mathcal{D}(\mathcal{A})$ are found such that the spectrum of $\mathcal{A}$ is a sequence of non-negative real numbers:

$$\lambda_k \geq 0, \quad k = 1, 2, \ldots.$$

Remark. *$\mathcal{D}(\mathcal{A})$, the domain of $\mathcal{A}$ consists of all $\psi \in \mathcal{H}$, where $\mathcal{A}\psi = \lambda\psi$ for some λ and moreover ψ satisfies boundary conditions in (4.1).*

The following lemma can be an appropriate means to investigate the long term behavior of the system.

Lemma 4.2. *If*

$$u = \sum_{k=1}^{\infty} a_k(t)\psi_k(x), \tag{4.3}$$

$$f = \sum_{k=1}^{\infty} f_k\psi_k(x), \tag{4.4}$$

satisfy problem (4.1), where $\psi_k(x) \in \mathcal{D}(\mathcal{A})$; then we have

$$a_k(t) = c_{1k}e^{{}^{+}r_k t} + c_{2k}e^{{}^{-}r_k t}, \tag{4.5}$$

$$f_k = -({}^{-}r_k c_{1k} + {}^{+}r_k c_{2k}), \tag{4.6}$$

in which

$$c_{1k} = \frac{(u_i, \varphi_k) - (u_0, \varphi_k)e^{{}^{-}r_k i}}{e^{{}^{+}r_k i} - e^{{}^{-}r_k i}}, \tag{4.7}$$

$$c_{2k} = \frac{-(u_i, \varphi_k) + (u_0, \varphi_k)e^{{}^{+}r_k i}}{e^{{}^{+}r_k i} - e^{{}^{-}r_k i}}, \tag{4.8}$$

for $i \in \{t_1, \ldots, t_N\}$, and

$${}^{+}r_k = \frac{-(\beta + \lambda_k) + \sqrt{\Delta_k}}{2}, \tag{4.9}$$

$${}^{-}r_k = \frac{-(\beta + \lambda_k) - \sqrt{\Delta_k}}{2}, \tag{4.10}$$

$$\Delta_k = (\beta + \lambda_k)^2 + 4\alpha. \tag{4.11}$$

Proof. Setting proposed u and f in (4.1), this PDE system is reduced to a set of ODEs:

$$\dot{a}_k(t) + a_k(t)(\lambda_k + \beta) - \alpha \int_0^t a_k(s)ds = f_k, \qquad k = 1, 2, \ldots, M. \tag{4.12}$$

Consequently we arrive

$$\ddot{a}_k(t) + \dot{a}_k(t)(\lambda_k + \beta) - \alpha a_k(t) = 0, \tag{4.13}$$

which results $a_k(t)$.

Now using $u_0(x)$ and $u_i(x)$ where $i \in \{t_1, \ldots, t_N\}$, the constants c_{1k} and c_{2k} are approximated. Introducing $a_k(t)$ in (4.12) we gain f_k. ∎

Theorem 4.3. *Assume that the Hypothesis* (H) *is satisfied, if* $\alpha < 0$ *and* $\beta > 2\sqrt{|\alpha|}$*, then any solution of the problem* (4.1) *decays to zero as* t *tends to infinity.*

Proof. Since it is known that the eigenfunctions span the function space containing the solution u, any solution of the problem (4.1) may be expanded as a Fourier series:

$$u(x,t) = \sum_{k=1}^{\infty} a_k(t)\psi_k(x). \tag{4.14}$$

From Lemma 4.2, we see that the coefficients $a_k(t)$ in (4.14) satisfy

$$a_k(t) = c_{1k}e^{{}^{+}r_k t} + c_{2k}e^{{}^{-}r_k t}, \qquad k = 1, 2, \ldots.$$

Now, $\alpha < 0$ and $\beta > 2\sqrt{|\alpha|}$ imply that $\sqrt{\Delta_k} < \beta + \lambda_k$. Hence, because $\lambda_k \geq 0$ we have ${}^{+}r_k < 0$ and ${}^{-}r_k < 0$, which impose $a_k(t)$ and consequently u approach zero as $t \to \infty$. ∎

An argument similar to what we have used in the proof of Theorem 4.3 leads to the following.

Theorem 4.4. *Assume that the Hypothesis* (H) *is satisfied, if* $\alpha = 0$ *and* $\beta > 0$*, then the solution of the problem* (4.1) *tends to the steady state* $u(x,t) = \sum_{k=1}^{\infty} c_{1k}\psi_k(x)$ *as* t *tends to infinity.*

Theorem 4.5. *Assume that the Hypothesis* (H) *is satisfied and* $\alpha > 0$*, then the solution of the problem* (4.1) *is strictly increasing.*

Since empirical eigenfunctions of the problem (4.1) computed through POD method can be used instead of the eigenfunctions of $\mathcal{A}$ [23], we can use the introduced theorems to study the long-term behavior of the system.

B. Galerkin Projection and Approximating Parameters

Let $\{\varphi_k \in \mathcal{H} \mid k = 1, \ldots, M\}$ be the orthonormal empirical eigenfunctions extracted by POD method described in the previous section where $M \leq N$ (N is the number of snapshots used in the POD method). The best M satisfies the inequality

$$\frac{\sum_{k=1}^{M} \lambda_k}{\sum_{k=1}^{N} \lambda_k} \geq 0.99.$$

However in general, eigenfunctions can be obtained analytically if it is possible. In any case, these functions can be an orthonormal basis to form a finite-dimensional subspace $\mathcal{S}_M$ of $\mathcal{H}$.

To apply Galerkin projection, we attempt to find the coordinates of the unknown parameters u and f of (4.1) with respect to this basis. Therefore we define the approximating solutions for u and f as two functions u_M and f_M, which belong to the finite-dimensional linear space $\mathcal{S}_M$ in the form:

$$u_M = \sum_{k=1}^{M} a_k(t)\varphi_k(x),$$

$$f_M = \sum_{k=1}^{M} f_k\varphi_k(x).$$

Now, from Lemma 4.2, f_k and the time-varying coordinate or coefficient $a_k(t)$ are determined. To recovery the nonlinear diffusion coefficient $D(C)$, defining

$$w(x,t) = \frac{\partial u}{\partial t} + v\frac{\partial u}{\partial x} - \alpha\int_0^t u(s)ds - f(x) + \beta u,$$

and considering (4.1), we will have

$$\frac{\partial}{\partial x}\left(D(C)\frac{\partial u}{\partial x}\right) = w(x,t).$$

Therefore, at any point in which $\partial u/\partial x \neq 0$, the following equation for identification D is valid:

$$D(C) = \frac{\int_{-1}^{x} w(s,t)ds}{\frac{\partial u}{\partial x}}.$$

Knowing the nonlinear diffusion coefficient at many distinguished points in Ω where $\partial u/\partial x \neq 0$ and different times, one can try and use an interpolation technique to find the solution that would approximate $D(C)$ for all positions and times. However, we must note that the interpolation found in this way is not unique, but for the purposes of current article quite satisfactory.

5. METHOD VALIDATION

To numerically test the described method, we present two numerical examples intended to demonstrate the usefulness of the approach. The test was performed using MATLAB, in IEEE double precision.

Example 1. The Linear Diffusion Case. As a simple example, let $D(C) = d$ be a constant and known value, and moreover the functions u and f belong to $\mathcal{S}$ exactly, i.e., f, $u \in \mathcal{S} = \text{span}\{\varphi_1, \varphi_2, \ldots\}$. Therefore, we consider

$$u(x,t) = \frac{\varphi_1(x)}{\sqrt{\Delta_1}}\left[e^{+r_1 t} + e^{-r_1 t}\right], \qquad f(x) = \varphi_1(x),$$

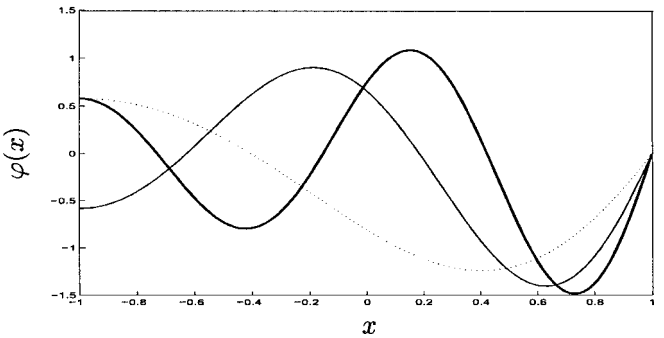

FIG. 1. First three eigenfunctions: φ_1 (solid thick line), φ_2 (solid thin line), and φ_3 (dashed line).

TABLE I. First six eigenvalues.

k	λ_k	k	λ_k
1	89.53267748568898	4	18.47151315026254
2	59.92386265801924	5	6.62795939292331
3	36.23680888457366	6	0.70582394728014

which exactly satisfy (4.1) for $D(C) = d$ with the boundary and initial conditions

$$\frac{\partial}{\partial x}u(-1,t) = 0,$$

$$u(1,t) = 0,$$

$$u_0(x) = \frac{2\varphi_1(x)}{\sqrt{\Delta_1}}.$$

Furthermore, to satisfy the condition $N \geq 1$ to solve the inverse problem, we consider

$$u_T(x) = \frac{\varphi_1(x)}{\sqrt{\Delta_1}}\left[e^{+r_1 T} + e^{-r_1 T}\right],$$

where T is an arbitrary positive number.

In this case that we have linearity in diffusion term, eigenfunctions can obtain analytically. Here, for simplicity in computations, we use (as it is permitted from [15]) the inner product

$$(\psi_1, \psi_2) = \int_\Omega \psi_1(x)\psi_2(x)e^{-(v/d)}dx,$$

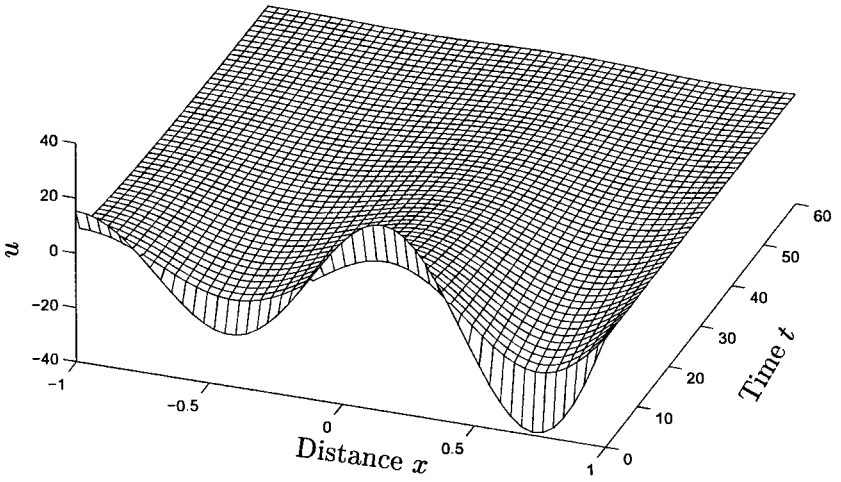

FIG. 2. u for $\alpha = -2$ and $\beta = 3$, approximated by three eigenfunctions.

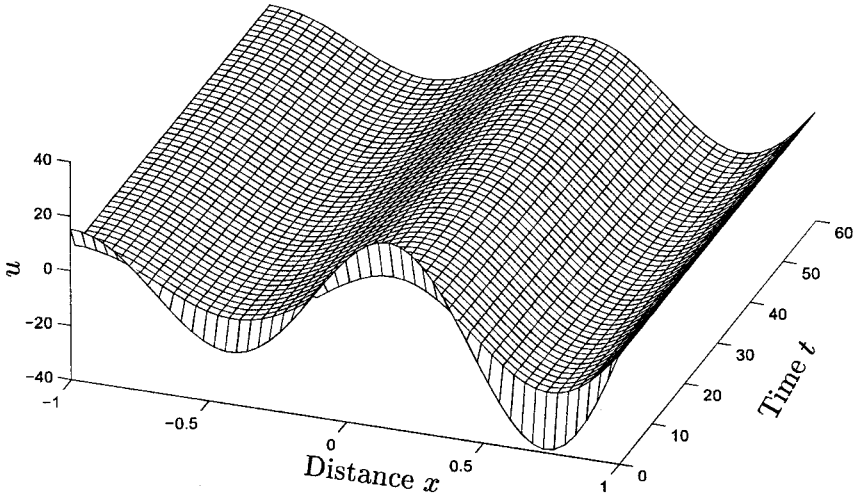

FIG. 3. u for $\alpha = 0$ and $\beta = 3$, approximated by three eigenfunctions.

for the elements of $\mathcal{H}$. Hence, we will have the orthonormal eigenfunctions and the corresponding eigenvalues as follows:

$$\{\varphi_j(x)\}_{j=1}^{\infty} = \left\{ \frac{\exp\left(\frac{v}{2d}x\right)\sin\left(\frac{w_j}{2}(x-1)\right)}{\sqrt{1-\frac{d}{v}\cos^2(w_j)}} \right\}_{j=1}^{\infty},$$

$$\{\lambda_j\}_{j=1}^{\infty} = \left\{ \frac{v^2}{4d} + \frac{d}{4}w_j^2 \right\}_{j=1}^{\infty},$$

such that w_j is a positive real number satisfying $v/d\tan(w_j) = w_j$.

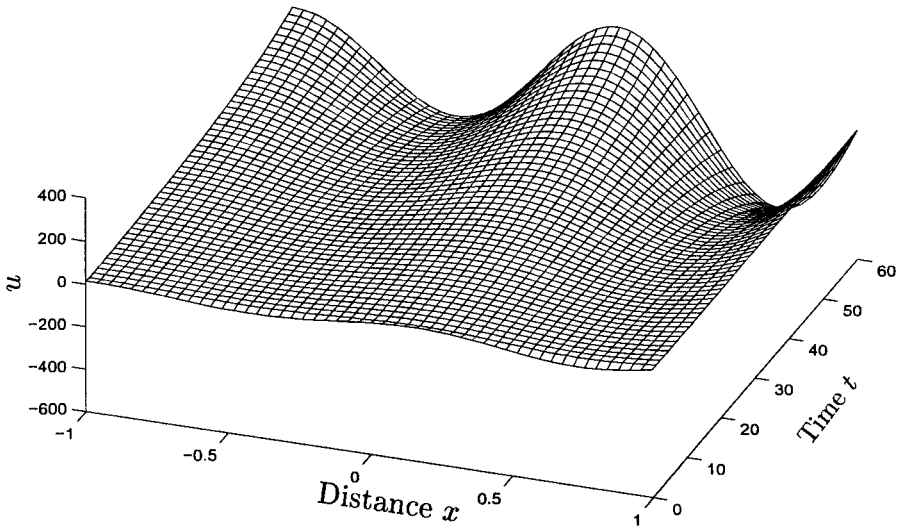

FIG. 4. u for $\alpha = 2$ and $\beta = 3$, approximated by three eigenfunctions.

Let $v = 0.07$ and $d = 1.2$. Figure 1 shows first three eigenfunctions, and Table I indicates first six eigenvalues, when we choose $N = 6$ and $M = 3$. Computed solutions u using these basis functions for different values α are illustrated by Figs. 2–4, which are in agreement with Theorem 4.3 and next two theorems. Figure 5 presents the high precision of the approximation procedure. Throughout Fig. 6 we see that using only three basis functions does not lead to a good approximation for $d = 1.2$. But increasing the number of approximating functions from 3 to 5 solves this problem.

Example 2. The nonlinear diffusion case. Here, as a nonlinear diffusion term we consider $D(C) = (1/\beta_1^2)e^{-2\alpha_1 t}C^2$ or equivalently $D(C) = u^2$. To generate computational data as snapshots and numerically test the POD-Galerkin method, the parameters in 4.1 are chosen as follows:

$$\alpha = 0, \qquad \beta = 1,$$
$$f(x) = x^2 + 2x - 3,$$
$$u_0(x) = \cos(x) - \cos(1) + (1 - x)\sin(1).$$

This PDE is solved using the spatial discretization method proposed in [24]. Figure 7 shows the system solution that can be used to produce empirical eigenfunctions. Employing the POD

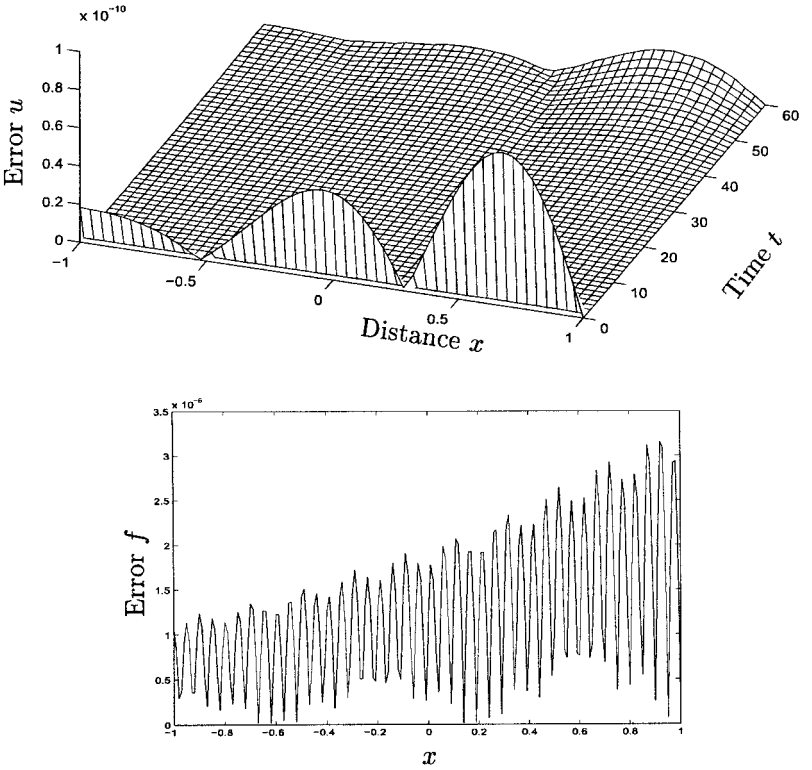

FIG. 5. Absolute difference between exact and approximated solution with three eigenfunctions for $\alpha = 2$ and $\beta = 3$: error u (top) and error f (bottom).

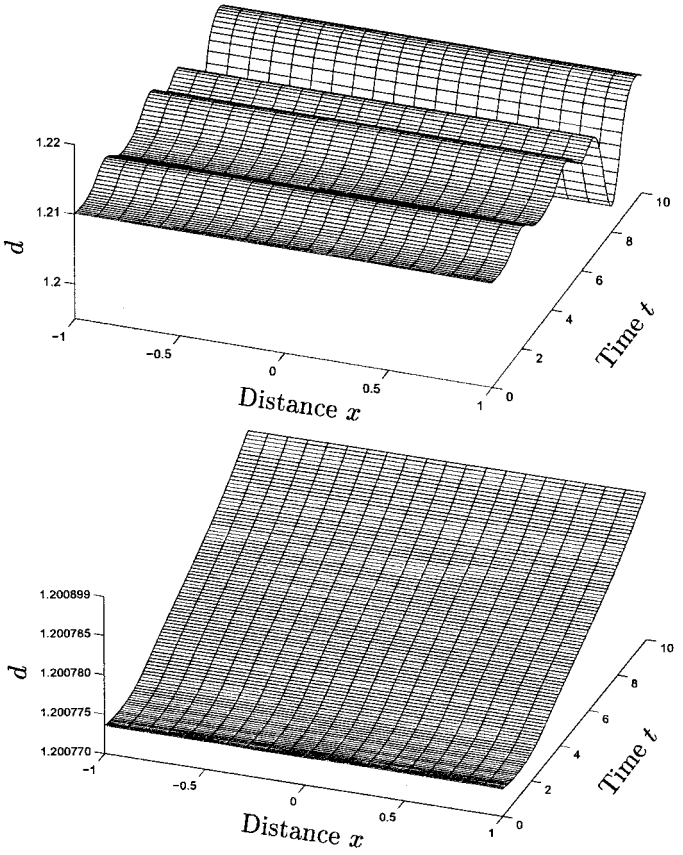

FIG. 6. Computed diffusion coefficient with three eigenfunctions (top) and five eigenfunctions (bottom).

technique on these computational data as snapshots results the empirical eigenfunctions, some of which are illustrated in Fig. 8, where corresponding eigenvalues are presented in Table II.

To apply the Galerkin method, all parameters are assumed to be known, except $f(x)$ and $D(C)$. Furthermore, we choose $N = 30$ and $M = 20$, which result very good approximations that can be observed from Figs. 9 and 10 and Table III.

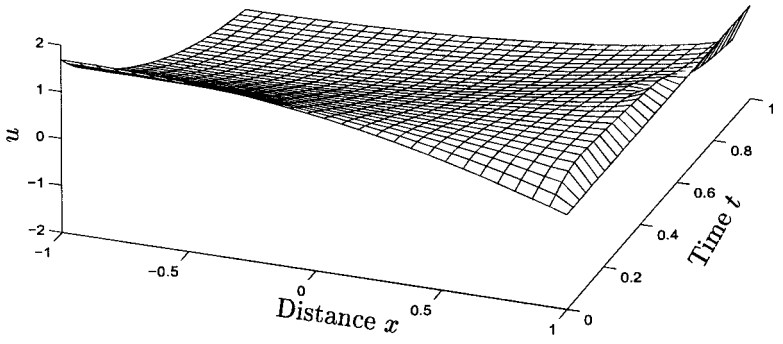

FIG. 7. u approximated by known parameters.

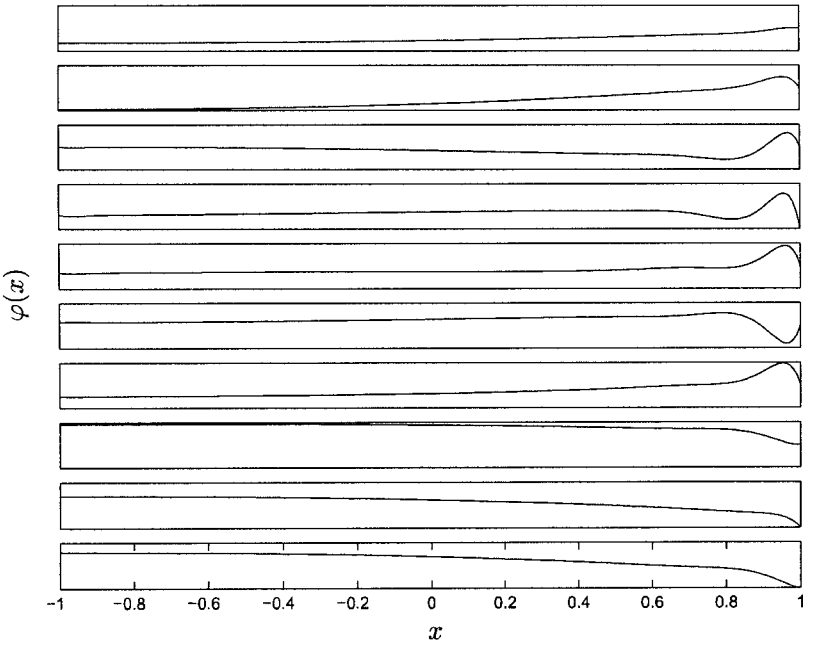

FIG. 8. First ten empirical eigenfunctions (φ_1 at the top of the figure).

TABLE II. The first 10 empirical eigenvalues.

k	λ_k	k	λ_k
1	1.37045566536630	6	0.00001275708375
2	0.02774251565115	7	0.00000995501297
3	0.01242094699976	8	0.00000642068196
4	0.00010082248651	9	0.00000566484412
5	0.00001594062844	10	0.00000399309204

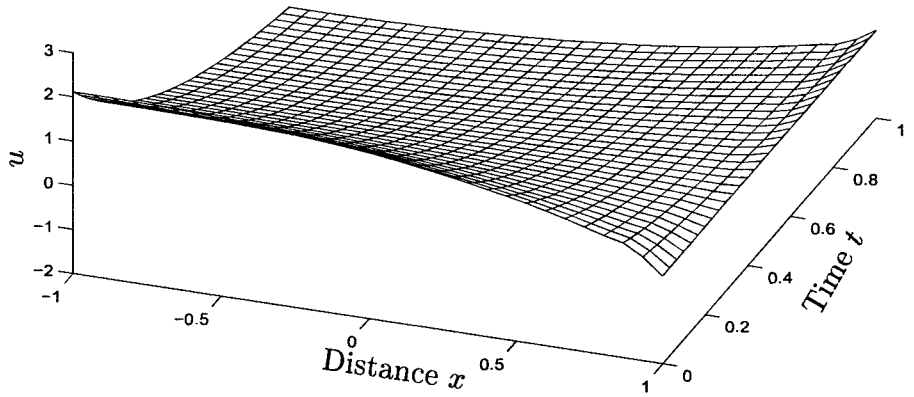

FIG. 9. u approximated by 20 empirical eigenfunctions.

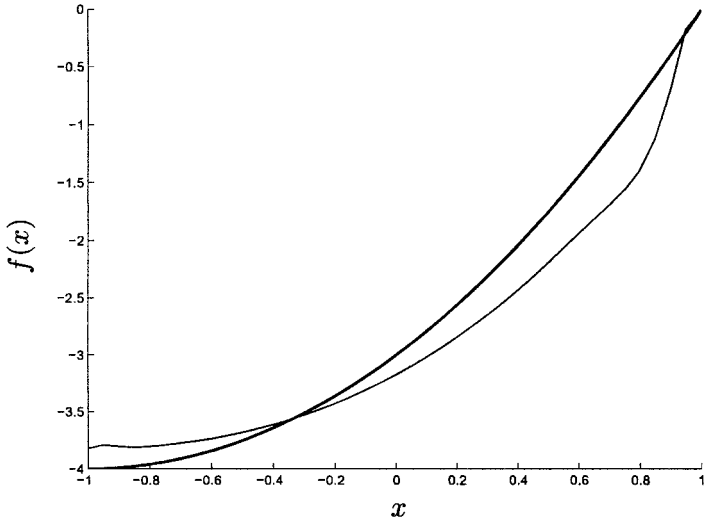

FIG. 10. Exact $f(x)$ (thick line) and approximated $f(x)$ (thin line).

6. SUMMARY AND CONCLUSIONS

We have considered a comprehensive transport model in which solute particles partition into two different phases: free particles and captured particles. Therefore, the model contains a diffusion-convection-reaction equation and a reaction process. To develop the model, we considered a nonlinear diffusion coefficient that is unknown and must be determined from observed or simulated data. In order to identify model unknowns such as free particles concentration, initial captured particles concentration, and diffusion coefficient, we have studied model order reduction applying a combination of the POD and Galerkin methods. The POD-Galerkin method yields very good and long-term predictions. Thus the long-term dynamics of the system have been studied from which some model parameters can be discussed. To validate the method, we have presented some numerical examples. Using a MATLAB program, it was found that in the linear diffusion case, only three POD modes or approximating functions can be sufficient to describe system dynamics and identify unknown parameters with reasonable accuracy. However, the diffusion coefficient

TABLE III. Nonlinear diffusion coefficient ($t = 0.1$).

x	Exact D(C)	Approximated D(C)	Absolute error
−0.6	1.1125	1.161	0.048489
−0.4	1.0603	1.2201	0.15981
−0.2	0.9832	1.0819	0.098699
0	0.88025	1.0457	0.16542
0.2	0.75163	0.94554	0.19391
0.4	0.59933	0.96182	0.36249
0.6	0.42956	0.94652	0.51696
0.8	0.28423	0.38481	0.10058
1	0	−0.77374	0.77374

may be approximated better using five approximating functions. In the nonlinear diffusion case, we must use more approximating functions to gain good results.

APPENDIX

Nomenclature

C	concentration in the mobile phase
C_s	concentration in the immobile phase
C^0	initial mobile concentration (a known function)
C_s^0	initial immobile concentration
D	diffusion coefficient
γ	a known function
ε	media porosity
v	velocity
ρ_s	media bulk density
ρ_b	solute density
R_{gf}	rate of growth (production) of freely suspended particles (cells)
R_{df}	rate of decay of freely suspended particles (cells)
R_{gs}	rate of growth of sessile particles (cells)
R_{ds}	rate of decay of sessile particles (cells)
R_r	rate of release of captured particles (cells)
R_c	rate of capture of suspended particles (cells)
k_{gf}	specific growth rate of free particles (cells)
k_{df}	specific decay rate of free particles (cells)
k_{gs}	specific growth rate of sessile particles (cells)
k_{ds}	specific decay rate of sessile particles (cells)
k_r	release rate coefficient for sessile particles (cells)
k_c	captured coefficient for freely suspended particles (cells)
x	distance
t	time
Ω	spatial domain
A	the ensemble averaged covariance matrix
$\mathcal{A}$	spatial differential operator
$\mathcal{D}(\mathcal{A})$	domain of $\mathcal{A}$
α	a constant
β	a constant
$L^2(\Omega)$	the space of square integrable functions defined in Ω
$\mathcal{H}$	a Hilbert space ($\mathcal{H} = L^2(\Omega)$)
$\langle\cdot\rangle$	temporal averaging operation
$(,)$	inner product
$\|.\|$	norm corresponding to $(,)$
u	state variable
u_t	snapshot
f	an unknown function
a_k	time-varying coefficient
ψ	some vector in $\mathcal{H}$
φ	eigenfunction (basis function)

λ	eigenvalue
N	number of snapshots
M	number of eigenfunctions employed

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