Original article

A reduced-order finite volume element formulation based on POD method and numerical simulation for two-dimensional solute transport problems[☆]

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Abstract

Proper orthogonal decomposition (POD) method has been successfully used in the reduced-order modeling of complex systems. In this paper, we extend the applications of POD method, i.e., combine the classical finite volume element (FVE) method with the POD method to obtain a reduced-order FVE formulation with lower dimensions and sufficiently high accuracy for two-dimensional solute transport problems, which have real life practical applications. We then provide error estimates between the reduced-order POD FVE solutions and classical FVE solutions and we provide implementation of an extrapolation algorithm for solving the reduced-order FVE formulation. Thus, we provide the theoretical basis for practical applications. A numerical example is then used to ascertain that the results of numerical computation are consistent with the theoretical derivations. Moreover, it is shown that the reduced-order FVE formulation based on POD method is both feasible and efficient for solving two-dimensional solute transport problems.
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1. Introduction

The solute in the soil is not only the essential condition for growing of agricultural crops, but is also related to the environmental pollution factor which grows as time goes by. The use of fertilizers and pesticides and the discharge

of industrial waste water could cause the increase in salinity and other organic or inorganic pollution materials in the soil. Their transport and accumulation leads to environmental degradation, resource reduction and degeneration of soil, and thus seriously affects the sustainable development of agricultural production and human health. The environment has become a major issue of concern to all the countries in the world. Therefore, research of solute transport along with effluents is closely related to preventing soil pollution, fully utilizing the available land resources, and improving agricultural production as well as protecting the environment.

The solute transport problems are mathematically described by a partial differential equation based on Darcy's law, which usually includes complex hydrodynamic dispersion coefficients, the average velocity of the water flow, and a source term which is dependent on water flow in the soil as well as soil types (see [5,17,29,61]). Therefore, finding their exact solutions for the practical solute transport problems is not an easy task. Thus, an efficient approach is to find their numerical solutions (see [19,35,34]).

The finite volume element (FVE) method (see [10,24,56]) is considered as one of the most effective numerical methods due to their following advantages. Firstly, it preserves the integral invariants of conservation of mass as well as that of total energy. Second, it has higher accuracy and is more suitable for computations involving complicated boundary conditions than the finite difference (FD) method. Third, it has the same accuracy as the finite element (FE) method but is simpler and more convenient to apply than the FE method. The FVE method is also known as a box method (see [4]) as an early reference where one discretised the integral form of conservation law of the differential equation by choosing a linear (or bilinear) FE space as the trial space. It is also referred to as a generalized difference method in China (see [31,32]). It has been widely applied to finding numerical solutions of different types of partial differential equations, for example, second order elliptic equations, parabolic equations, and Stokes equations (see [4,7,10,14,15,19,24,30–32,35,54,34,56,59,60]).

Though some classical fully discrete FVE formulations for two-dimensional solute transport problems are more effective than their FE formulations and FD schemes (see for instance, the material in [19,34,35]), they include too many degrees of freedom. Thus, an important problem is how to reduce the number of degrees of freedom and thus alleviate the computational load and save CPU time. This is done in a manner that guarantees a sufficiently accurate numerical solution.

It has been shown that the proper orthogonal decomposition (POD) method by combining with numerical methods for solving partial differential equations can provide an efficient means of generating reduced-order models and alleviate the computational load as well as memory requirements (see [22]). The POD method has been widely and successfully applied to numerous fields, including signal analysis and pattern recognition (see [20]), statistics (see [23]), geophysical fluid dynamics or meteorology (also see [23]). The POD method essentially provides an orthogonal basis for representing the given data in a certain least squares optimal sense, that is, it provides a way to find an optimal lower dimensional approximation of the given data.

In early applications, the POD method was mainly used to perform principal component analysis in computations of statistics and find the main behavior of a dynamical system (see [3,6,13,22,23,25,36,46,47,51–53]), until the method of snapshots was introduced by Sirovich (see [55]). Then the POD method was widely applied to reducing the order of the POD eigenvalue problem. Until ten years ago, the Galerkin POD methods for parabolic problems as well as a general equation in fluid dynamics have not been presented as yet (see [26,27]). Also the singular value decomposition approach combined with POD technique has not been yet used to treat the Burgers equation (see [28]) and the cavity flow problem (see [2]). More recently, a number of reduced-order FD models and FE (or mixed FE or least-square mixed FE) formulations and error estimates for the upper tropical Pacific Ocean model, parabolic problems, Burgers equation, the non-stationary Navier–Stokes equations, the non-stationary conduction–convection problems, and CVD equations based on POD method were presented by our research group (see [11,12,38–45,57,58]). Moreover, there are some reduced basis methods (combined with the POD method) for incompressible viscous/parabolic flows that play an important role in reducing the number of degrees of freedom and save time-consuming calculations along with resource demands (see [9,18,21,48–50]).

Though a reduced basis method for FVE approximations of parameterized linear evolution equations has been presented (see [21]) and a reduced FE formulation based POD method for two-dimensional solute transport problems has been posed in [33], to the best of our knowledge, there are no published results addressing the case where a combination of the POD method with FVE methods is used to deal with the two-dimensional solute transport problems or providing estimates of the error between classical FVE solutions and reduced-order FVE solutions. In this paper, we extend the developments in [21,33], i.e., establish a reduced-order FVE formulation with lower dimensions and

sufficiently high accuracy based on FVE method and POD method for the two-dimensional solute transport problems with real-life applications, analyze the errors between the reduced-order FVE solutions and the classical FVE solutions, and provide the implementation of the extrapolation algorithm for solving the reduced-order FVE formulation. Thus, we supply the theoretical basis for real implementation. A numerical example illustrates the fact that the results of the numerical computation are consistent with the theoretical results. Moreover, it is shown that the reduced-order FVE formulation based on POD method is both feasible and efficient for solving two-dimensional solute transport problems.

The rest of this paper is organized as follows. Section 2 derives the classical fully discrete FVE formulation for two-dimensional solute transport problems and discusses how to generate snapshots from the first few numerical solutions computed from the equation system derived by the classical fully discrete FVE formulation. In Section 3, the optimal orthonormal POD basic is reconstructed from the elements of the snapshots using POD method and a reduced-order FVE formulation for two-dimensional solute transport problems is established. In Section 4, we provide the error estimates between the classical FVE solutions and the reduced-order FVE solutions along with the implementation of extrapolation algorithm for solving the reduced-order FVE formulation. In Section 5, a numerical example is presented illustrating that the numerically computational errors between the reduced-order FVE approximate solutions and the classical FVE solutions are consistent with the previously obtained theoretical results, thus validating the feasibility and efficiency of the reduced-order FVE formulation. Section 6 sums-up the main conclusions and discusses future tentative research ideas.

2. A classical fully discrete FVE formulation for two-dimensional solute transport problems and generation of snapshots

According to the convection and hydrodynamic dispersion (molecular diffusion and mechanical dispersion), the two-dimensional solute transport model (see [29]) can be described as follows.

Problem I. Find c such that

$$\begin{cases} c_t - (D_1(\boldsymbol{v}, \theta)c_x)_x - (D_2(\boldsymbol{v}, \theta)c_y)_y + (q_1 c)_x + (q_2 c)_y = S_r, & (x, y) \in \Omega, \quad t \in (0, T), \\ c(x, y, 0) = c_0(x, y), & (x, y) \in \Omega, \\ c(x, y, t) = c_\Gamma(x, y, t), & (x, y) \in \Gamma, \quad t \in (0, T), \end{cases} \tag{2.1}$$

where $\Omega \subset \mathbb{R}^2$ represents a bounded, connected, and polygonal domain, $c(x, y, t)$ the solute density at point (x, y) in Ω and time t, θ the soil moisture density, $\boldsymbol{v} = \boldsymbol{q}\theta^{-1}$ ($\boldsymbol{q} = (q_1, q_2)$) the average hole velocity of water flow, S_r the solute producing or vanishing in the unit time and in the unit volume soil, T total time, $\Gamma = \partial\Omega$, q_1 and q_2 are water fluxes at x-direction and y-direction, respectively, $D_1(\boldsymbol{v}, \theta)$ and $D_2(\boldsymbol{v}, \theta)$ are hydrodynamic dispersion coefficients at x-direction and y-direction (which is the vertical direction, i.e., positive downward), respectively, $c_0(x, y)$ and $c_\Gamma(x, y, t)$ are two given functions. For the sake of convenience, without loss of generality, we may as well suppose that $c_\Gamma(x, y, t) = c_0(x, y) = 0$ in the following theoretical analysis.

The Sobolev spaces used in this context are standard (see [1]). Let $U = H_0^1(\Omega)$ be a Hilbert space on real field Ω. Then, the variational formulation for Problem I can be written as follows.

Problem II. Find $c(t): [0, T] \to U$ such that

$$\begin{cases} (c_t, w) + a(c, w) - b(c, w) = (S_r, w), & \forall w \in U, \\ c(x, y, 0) = 0, & (x, y) \in \Omega, \end{cases} \tag{2.2}$$

where $a(c, w) = (D_1(\boldsymbol{v}, \theta)c_x, w_x) + (D_2(\boldsymbol{v}, \theta)c_y, w_y)$, $b(c, w) = (c, \boldsymbol{q}\nabla w)$, $(\cdot, \cdot)$ denotes the inner product in $L^2(\Omega)$.

In order to obtain the numerical solution of FVE formulation for Problem II, it is necessary to introduce a FVE approximation for the spatial variables of Problem II.

First, let $\mathfrak{I}_h = \{K\}$ be a quasi-uniform triangulation of Ω with $h = \max h_K$, where h_K is the diameter of the triangle $K \in \mathfrak{I}_h$ (see [4,10,30,31,54,56,59]). In order to describe the FVE method, we shall introduce a dual partition $\mathfrak{I}_h^*$ based on $\mathfrak{I}_h$ whose elements are called the control volumes. We construct the control volume in the same way as in
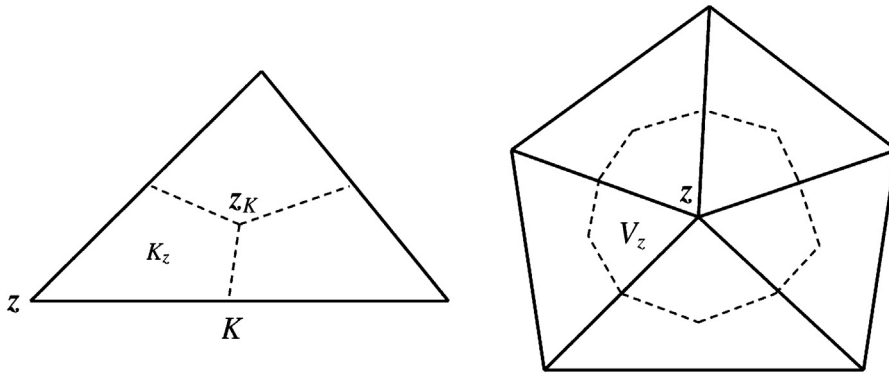
Fig. 1. Left-hand side: A triangle K partitioned into three sub-regions K_z. Right-hand side: A sample region with dotted lines indicating the corresponding control volume V_z.

[4,10,31,56]. Let z_K be the barycenter of $K \in \mathfrak{I}_h$. We connect z_K with line segments to the midpoints of the edges of K, thus partitioning K into three quadrilaterals K_z ($z = (x_z, y_z) \in Z_h(K)$, where $Z_h(K)$ are the vertices of K). Then with each vertex $z \in Z_h = \bigcup_{K \in \mathfrak{I}_h} Z_h(K)$ we associate a control volume V_z, which consists of the union of the sub-regions K_z, sharing the vertex z. Finally, we obtain a group of control volumes covering the domain Ω, which is called the dual partition $\mathfrak{I}_h^*$ of the triangulation $\mathfrak{I}_h$ (see Fig. 1). We denote the set of interior vertices of Z_h by Z_h°.

We call the partition $\mathfrak{I}_h^*$ regular or quasi-uniform, if there exist two positive constants $\widetilde{M}_1$ and $\widetilde{M}_2$, being independent of the spatial mesh size h and temporal mesh size, such that

$$\widetilde{M}_1 h^2 \leq \mathrm{mes}(V_z) \leq \widetilde{M}_2 h^2, \quad \forall V_z \in \mathfrak{I}_h^*, \tag{2.3}$$

where $\mathrm{mes}(V_z)$ denotes the measurement of control volume element V_z. The barycenter-type dual partition can be introduced for any FE triangulation $\mathfrak{I}_h$ and leads to relatively simple calculations. Besides, if the FE triangulation $\mathfrak{I}_h$ is quasi-uniform, then the dual partition $\mathfrak{I}_h^*$ is also quasi-uniform (see [4,8,10,16,31,32,37,56]).

The trial function space U_h chosen as the linear element space related to $\mathfrak{I}_h$ is the set of all the functions w_h satisfying the following conditions:

(i) $w_h \in C(\overline{\Omega})$, $w_h|_{\partial\Omega} = 0$;
(ii) $w_h|_K \in \mathcal{P}_1$, namely w_h is a linear function of x and y on each triangular element $K \in \mathfrak{I}_h$, determined only by its values on the three vertices.

It is obvious that $U_h \subset U = H_0^1(\Omega)$. For $w \in U = H_0^1(\Omega)$, let $\Pi_h w$ be the interpolation projection of w onto the trial function space U_h. By the interpolation theory of Sobolev spaces (see [4,10,8,16,31,32,37,56]), we have, if $w \in H^2(\Omega)$, that

$$|w - \Pi_h w|_m \leq M h^{2-m} |w|_2, \quad m = 0, 1, \tag{2.4}$$

where M in this context indicates a positive constant which is possibly different at different occurrences, being independent of the spatial mesh size h and the temporal mesh size.

The test space $\tilde{U}_h$ is chosen as the piecewise constant function space with respect to $\mathfrak{I}_h^*$ but is zero on any boundary dual element $V_z \in \mathfrak{I}_h^*$, i.e.,

$$\tilde{U}_h = \{w_h \in L^2(\Omega); \quad w_h|_{V_z} \in \mathcal{P}_0(V_z), \quad \forall V_z \in \mathfrak{I}_h^*, w_h|_{V_z} = 0, \quad \text{on any boundary dual element} \quad V_z\}$$

spanned by the following basis functions: for any point $z \in Z_h^\circ$,

$$\phi_z(x, y) = \begin{cases} 1, & (x, y) \in V_z, \\ 0, & \text{elsewhere.} \end{cases} \tag{2.5}$$

For any $w_h \in \tilde{U}_h$,

$$w_h = \sum_{z \in Z_h^\circ} w_h(z)\phi_z. \tag{2.6}$$

For $w \in U$, let $\Pi_h^* w$ be the interpolation projection of w onto the test space $\tilde{U}_h$, i.e.,

$$\Pi_h^* w = \sum_{z \in Z_h^\circ} w(z)\phi_z. \tag{2.7}$$

By the interpolation theory (see [8,16,31,37]), we have

$$\|w - \Pi_h^* w\|_0 \le Mh|w|_1. \tag{2.8}$$

Moreover, the interpolation projection Π_h^* satisfies the following properties (see [31]).

Lemma 1. *If* $v_h \in U_h$, *then*

$$\int_K (v_h - \Pi_h^* v_h)\mathrm{d}x\,\mathrm{d}y = 0, \quad K \in \mathfrak{I}_h; \quad \|v_h - \Pi_h^* v_h\|_{L^r(\Omega)} \le Mh_K \|v_h\|_{W^{1,r}(\Omega)}, 1 \le r \le \infty.$$

Though the trial function space U_h satisfies $U_h \subset U$ like FE methods, the test space $\tilde{U}_h \not\subset U_h$. As in the case of nonconforming FE methods, this is due to the loss of continuity of the functions in $\tilde{U}_h$ on the boundary of two neighboring elements. So the bilinear forms $a(c, w)$ must be revised accordingly. Using the idea of nonconforming FE methods, the integral on the whole region is written as a sum of the integrals on every element K, $a(c, w)$ of (2.2) is rewritten as

$$a(c, w) = \sum_{K \in \mathfrak{I}_h} \int_K \left(D_1(\boldsymbol{v}, \theta)\frac{\partial c}{\partial x}\frac{\partial w}{\partial x} + D_2(\boldsymbol{v}, \theta)\frac{\partial c}{\partial y}\frac{\partial w}{\partial y} \right) \mathrm{d}x\,\mathrm{d}y. \tag{2.9}$$

Now $a(c, w)$ is well-defined on $U_h \times \tilde{U}_h$. For the FVE methods, i.e., generalized difference methods, we place a dual grid and interpret (2.9) in the sense of generalized functions, i.e., δ functions on the boundary of neighboring dual elements. Or equivalently, we take $a(c, w)$ as the bilinear form resulting from the piecewise integrations by parts on the dual elements V_z:

$$\int_\Omega \left[\frac{\partial}{\partial x}\left(D_1 \frac{\partial c}{\partial x} \right) + \frac{\partial}{\partial y}\left(D_2 \frac{\partial c}{\partial y} \right) \right] w \mathrm{d}x\,\mathrm{d}y = \sum_{V_z \in \mathfrak{I}_h^*} \int_{V_z} \left[\frac{\partial}{\partial x}\left(D_1 \frac{\partial c}{\partial x} \right) + \frac{\partial}{\partial y}\left(D_2 \frac{\partial c}{\partial y} \right) \right] w \mathrm{d}x\,\mathrm{d}y$$

$$= -\sum_{V_z \in \mathfrak{I}_h^*} \int_{V_z} \left[D_1 \frac{\partial c}{\partial x}\frac{\partial w}{\partial x} + D_2 \frac{\partial c}{\partial y}\frac{\partial w}{\partial y} \right] \mathrm{d}x\,\mathrm{d}y + \sum_{V_z \in \mathfrak{I}_h^*} \int_{\partial V_z} \left(D_1 \frac{\partial c}{\partial x} w \mathrm{d}y - D_2 \frac{\partial c}{\partial y} w \mathrm{d}x \right), \tag{2.10}$$

where $\int_{\partial V_z}$ denotes the line integrals, with the counter clockwise direction, on the boundary ∂V_z of the dual element V_z. So we have

$$a(c, w) = \sum_{V_z \in \mathfrak{I}_h^*} \int_{V_z} \left[D_1 \frac{\partial c}{\partial x}\frac{\partial w}{\partial x} + D_2 \frac{\partial c}{\partial y}\frac{\partial w}{\partial y} \right] \mathrm{d}x\,\mathrm{d}y$$

$$- \sum_{V_z \in \mathfrak{I}_h^*} \int_{\partial V_z} \left(D_1 \frac{\partial c}{\partial x} w \, \mathrm{d}y - D_2 \frac{\partial c}{\partial y} w \, \mathrm{d}x \right), \quad \forall c, \quad w \in U. \tag{2.11}$$

Since $\tilde{U}_h$ is the piecewise constant function space with the characteristic functions of the dual elements V_z as the basis functions, then

$$
\begin{aligned}
a(c_h, w_h) &= -\sum_{V_z \in \mathfrak{I}_h^*} \int_{\partial V_z} \left(D_1 \frac{\partial c_h}{\partial x} w_h \mathrm{d}y - D_2 \frac{\partial c_h}{\partial y} w_h \mathrm{d}x \right) \\
&= -\sum_{V_z \in \mathfrak{I}_h^*} w_h(z) a(c_h, \phi_z), \qquad \forall c_h \in U_h, \quad \forall w_h \in \tilde{U}_h,
\end{aligned}
\tag{2.12}
$$

where $a(c_h, \phi_z) = \int_{\partial V_z} \left(\frac{D_1 \partial c_h}{\partial x} \mathrm{d}y - \frac{D_2 \partial c_h}{\partial y} \mathrm{d}x \right)$.

Similarly, we have that

$$
b(c_h, w_h) = -\sum_{V_z \in \mathfrak{I}_h^*} \int_{\partial V_z} (q_1 c_h w_h \mathrm{d}y - q_2 c_h w_h \mathrm{d}x) = -\sum_{V_z \in \mathfrak{I}_h^*} w_h(z) b(c_h, \phi_z), \quad \forall c_h \in U_h, \quad \forall w_h \in \tilde{U}_h, \tag{2.13}
$$

where $b(c_h, \phi_z) = \int_{\partial V_z} (q_1 c_h \mathrm{d}y - q_2 c_h \mathrm{d}x)$.

Let τ denote the time step size, and let $c_h^n \in U_h$ be the fully discrete approximation to $c(t)$ at $t_n = n\tau$ ($n = 0, 1, \ldots, N = [T/\tau]$). If the differential quotient c_t in Problem II is approximated with the backward difference quotient $\bar{\partial}_t c^n = (c^n - c^{n-1})/\tau$ at time $t = t_n$, then the fully discrete FVE approximate scheme of Euler backward one step of Problem II about time reads as follows.

Problem III. Find $c_h^n \in U_h$ ($1 \le n \le N$) such that

$$
\begin{cases}
(c_h^n, \Pi_h^* w_h) + \tau a(c_h^n, \Pi_h^* w_h) - \tau b(c_h^n, \Pi_h^* w_h) = \left(c_h^{n-1}, \Pi_h^* w_h \right) + \tau(S_r^n, \Pi_h^* w_h), \quad \forall w_h \in U_h, \\
c_h^0 = 0, \quad (x, y) \in \Omega.
\end{cases}
\tag{2.14}
$$

The existence and uniqueness of solution of the variational Problem II and fully discrete FVE formulations, i.e., Problem III are proved and the following theorem of error estimates has been provided in [34] and is obtained by using the same approach as in the proofs for parabolic equations in [31].

Theorem 2. If $S_r \in L^2(\Omega)$ and there exist two constants $M_i > 0 (i = 1, 2)$ such that $D_1(\boldsymbol{v}, \theta)$, $D_2(\boldsymbol{v}, \theta)$, and $\boldsymbol{q}$ satisfy

$$
M_1 \le D_1(\boldsymbol{v}, \theta), D_2(\boldsymbol{v}, \theta), |\boldsymbol{q}| \le M_2, \tag{2.15}
$$

then there are the following error estimates between the solution c of Problem II and the solution c_h^n of Problem III:

$$
\|c(t_n) - c_h^n\|_0 \le M(h^2 + \tau), \quad n = 1, 2, \ldots, N, \tag{2.16}
$$

$$
\|c(t_n) - c_h^n\|_1 \le M(h + \tau), \quad n = 1, 2, \ldots, N, \tag{2.17}
$$

where M is a constant independent of h and τ but dependent on other data and S_r of Problem II.

If S_r, $D_1(\boldsymbol{v}, \theta)$, $D_2(\boldsymbol{v}, \theta)$, $\boldsymbol{q}$, the triangulation parameter h, the time step increment τ, and trial function space U_h are given, we can obtain a set of solution $\{c_h^n(x, y)\}_{n=1}^N$ by solving Problem III. And then we choose the first L (in general, $L \ll N$, for example, $L = 20$, $N = 200$) instantaneous solutions $c_h^i(x, y)$ ($1 \le i \le L$) (which are useful and of interest for us and at least one of which is assumed to be non-zero) from N instantaneous solutions $c_h^n(x, y)$ ($1 \le n \le N$) for Problem III, which are referred to as snapshots.

Remark 1. When one computes actual problems, one may obtain the ensemble of snapshots from physical system trajectories by drawing samples from experiments and interpolation (or data assimilation). For example, for real-life practical solute transport forecast, one can use the previously given solute transport results to construct the ensemble of snapshots, then reconstruct the POD optimal basis for the ensemble of snapshots by using the following POD method, and finally the trial function space U_h is substituted with the subspace generated with POD basis in order to derive a reduced-order dynamical system with a lower dimension. Thus, the future change of solute transport can be quickly simulated, which is of great practical value in real-life applications.

3. Generation of POD basis and reduced-order FVE formulation based on POD technique for Problem III

In this section, we cite the idea in Ref. [33] to generate a POD basis (more details see [33]) and establish a reduced-order FVE formulation based on POD technique for Problem III.

For $c_h^i(x, y)$ ($1 \le i \le L$) in Section 2, let $W_i(x, y) = c_h^i(x, y)$ ($1 \le i \le L$) and

$$\mathcal{V} = \text{span}\{W_1, W_2, \ldots, W_L\}, \tag{3.1}$$

and refer to $\mathcal{V}$ as the space generating by the snapshots $\{W_i\}_{i=1}^L$ at least one of which is assumed to be non-zero. Let $\{\psi_j\}_{j=1}^l$ denote an orthonormal basis of $\mathcal{V}$ with $l = dim\mathcal{V}$. Then each member of the ensemble can be expressed as

$$W_i = \sum_{j=1}^l (W_i, \psi_j)_U \psi_j, \quad i = 1, 2, \ldots, L, \tag{3.2}$$

where $(W_i, \psi_j)_U = (\nabla c_h^i, \nabla \psi_j)$.

Definition 1. The method of POD consists in finding the orthonormal basis ψ_j ($i = 1, 2, \ldots, l$) such that for every d ($1 \le d \le l$) the mean square error between the elements W_i ($1 \le i \le L$) and corresponding dth partial sum of (3.2) is minimized on average

$$\min_{\{\psi_j\}_{j=1}^d} \frac{1}{L} \sum_{i=1}^L \left\| W_i - \sum_{j=1}^d (W_i, \psi_j)_U \psi_j \right\|_U^2 \tag{3.3}$$

subject to

$$(\psi_i, \psi_j)_U = \delta_{ij}, \quad 1 \le i \le d, 1 \le j \le i, \tag{3.4}$$

where $\|W_i\|_U^2 = \|\nabla c_h^i\|_0^2$. A solution $\{\psi_j\}_{j=1}^d$ of (3.3) and (3.4) is known as a POD basis of rank d.

By (3.2) and orthonormality of ψ_j, we can rewrite (3.3) as follows.

$$\frac{1}{L} \sum_{i=1}^L \left\| W_i - \sum_{j=1}^d (W_i, \psi_j)_U \psi_j \right\|_U^2 = \frac{1}{L} \sum_{i=1}^L \left\| \sum_{j=d+1}^l (W_i, \psi_j)_U \psi_j \right\|_U^2 = \sum_{j=d+1}^l \left[\frac{1}{L} \sum_{i=1}^L \left| (W_i, \psi_j)_U^2 \right| \right]. \tag{3.5}$$

Thus, in order to assure that (3.5) is minimum, it is equivalent to find the orthonormal basis ψ_j ($j = 1, 2, \ldots, l$) such that

$$\max_{\{\psi_j\}_{j=1}^d} \sum_{j=1}^d \left[\frac{1}{L} \sum_{i=1}^L \left| (W_i, \psi_j)_U^2 \right| \right] \tag{3.6}$$

subject to

$$(\psi_i, \psi_j)_U = \delta_{ij}, \quad 1 \le i \le d, 1 \le j \le i. \tag{3.7}$$

In other words, (3.3) and (3.4) are equivalent to looking for a function ψ, or the so-called POD basis element, that most resembles $\{W_i(x)\}_{i=1}^L$ meaning that it maximizes

$$\frac{1}{L} \sum_{i=1}^L \left| (W_i, \psi)_U \right|^2 \quad \text{subject to} \quad (\psi, \psi)_U = \|\nabla \psi\|_0^2 = 1. \tag{3.8}$$

We cite the idea of snapshots introduced by Sirovich in [55] and choose a special class of trial function for ψ to be of the form:

$$\psi = \sum_{i=1}^L a_i W_i, \tag{3.9}$$

where the coefficients a_i are to be determined so that ψ given by the expression (3.9) provides a maximum for (3.8). Thus, (3.8) is equivalent to the eigenvalue problem

$$\boldsymbol{A}\boldsymbol{v} = \lambda \boldsymbol{v}, \tag{3.10}$$

where $\boldsymbol{A} = (A_{ik})_{L \times L}$ and

$$A_{ik} = \frac{1}{L} \int_{\Omega} \nabla W_i(x, y) \cdot \nabla W_k(x, y) \mathrm{d}x\,\mathrm{d}y, \quad \boldsymbol{v} = (a_1, a_2, \ldots, a_L)^T, \tag{3.11}$$

and λ depends on h and τ due to $\mathcal{V}$ depending on them. Since the matrix $\boldsymbol{A}$ is a nonnegative Hermitian matrix which has rank l, it has a complete set of orthonormal eigenvectors

$$\boldsymbol{v}^1 = (a_1^1, a_2^1, \ldots, a_L^1)^T, \quad \boldsymbol{v}^2 = (a_1^2, a_2^2, \ldots, a_L^2)^T, \ldots, \boldsymbol{v}^l = (a_1^l, a_2^l, \ldots, a_L^l)^T \tag{3.12}$$

with the corresponding eigenvalues $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_l > 0$. Thus, the solution to the optimization for (3.3) is given by

$$\psi_1 = \frac{1}{\sqrt{L\lambda_1}} \sum_{j=1}^{L} a_j^1 W_j, \tag{3.13}$$

where a_j^1 $(j = 1, 2, \ldots, L)$ are the elements of the eigenvector $\boldsymbol{v}^1$ corresponding to the largest eigenvalue λ_1. The remaining POD basis elements ψ_i $(i = 2, 3, \ldots, l)$ are obtained by using the elements of the other eigenvectors $\boldsymbol{v}^i$ $(i = 2, 3, \ldots, l)$, i.e.,

$$\psi_i = \frac{1}{\sqrt{L\lambda_i}} \sum_{j=1}^{L} a_j^i W_j. \tag{3.14}$$

Moreover, the POD basis $\{\psi_1, \psi_2, \ldots, \psi_l\}$ forms an orthonormal set and there holds the following result (see [26,38,39,55]).

Proposition 3. *Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_l > 0$ denote the positive eigenvalues of $\boldsymbol{A}$ and $\boldsymbol{v}^1, \boldsymbol{v}^2, \ldots, \boldsymbol{v}^l$ the associated orthonormal eigenvectors. Then a POD basis of rank $d \leq l$ is given by*

$$\psi_i = \frac{1}{\sqrt{L\lambda_i}}(W_1, W_2, ..., W_l) \cdot \boldsymbol{v}^i = \frac{1}{\sqrt{L\lambda_i}} \sum_{j=1}^{L} a_j^i W_j, \quad 1 \leq i \leq d \leq l. \tag{3.15}$$

Furthermore, the following error formula holds

$$\frac{1}{L} \sum_{i=1}^{L} \| W_i - \sum_{j=1}^{d} (W_i, \psi_j)_U \psi_j \|_U^2 = \sum_{j=d+1}^{l} \lambda_j. \tag{3.16}$$

Let $U^d = \mathrm{span}\{\psi_1, \psi_2, \ldots, \psi_d\}$. For $c \in U$, define the Generalized Ritz-projection $P^h : U \to U_h$ (if P^h is restricted to Ritz-projection from U_h to U^d, it is written as P^d) such that $P^h|_{U_h} = P^d : U_h \to U^d$ and $P^h : U \setminus U_h \to U_h \setminus U^d$ denoted by

$$a(P^h c, w_h) = a(c, w_h), \quad \forall w_h \in U_h, \tag{3.17}$$

where $c \in U$. Due to (3.17) the operator P^h is well-defined and bounded (see [59])

$$\|\nabla(P^h c)\|_0 \leq \frac{M_1}{M_2} \|\nabla c\|_0, \quad \forall c \in U \tag{3.18}$$

and the following inequality (see [38,39,59])

$$\|c - P^h c\|_0 \leq Mh \|\nabla(c - P^h c)\|_0, \qquad \forall c \in U. \tag{3.19}$$

And there hold the following results (see [26,38,39]).

Lemma 4. *For every d ($1 \le d \le l$), the projection operator P^d satisfies*

$$\frac{1}{L}\sum_{i=1}^{L}\|\nabla(c_h^i - P^d c_h^i)\|_0^2 \le \frac{M_1}{M_2}\sum_{j=d+1}^{l}\lambda_j, \tag{3.20}$$

where $c_h^i \in \mathcal{V}$ is the solution of Problem III. $\square$

Thus, by using U^d, we can obtain the reduced-order formulation based on POD for Problem III as follows.

Problem IV. Find $c_d^n \in U^d$ ($1 \le n \le N$) such that

$$\begin{cases} (c_d^n, \Pi_h^* w_d) + \tau a(c_d^n, \Pi_h^* w_d) - \tau b(c_d^n, \Pi_h^* w_d) = \left(c_d^{n-1}, \Pi_h^* w_d\right) + \tau(S_r^n, \Pi_h^* w_d), & \forall w_d \in U^d, \\ c_d^0 = 0, \quad (x, y) \in \Omega. \end{cases} \tag{3.21}$$

Let $c_d^n = \alpha_1^n \psi_1 + \alpha_2^n \psi_2 + \cdots + \alpha_d^n \psi_d$ ($n = 0, 1, \ldots, N$). By definition of Π_h^*, Problem IV can be rewritten as follows.

Problem V. Find $(\alpha_1^n, \alpha_2^n, \ldots, \alpha_d^n) \in R^d$ ($n = 1, 2, \ldots, N$) such that

$$\sum_{j=1}^{d}\alpha_j^n[B_{ij} + \tau C_{ij} + \tau Q_{ij}] = F_i^n + \sum_{j=1}^{d}\alpha_j^{n-1}B_{ij}, \quad i = 1, 2, \ldots, d, \tag{3.22}$$

where $\alpha_i^0 = 0$ ($i = 1, 2, \ldots, d$) and

$$F_i^n = \sum_{V_z \in \mathfrak{I}_h^*} \psi_i(x_z, y_z)\int_{V_z} S_r(x, y, t_n)\mathrm{d}x\,\mathrm{d}y, \quad B_{ij} = \sum_{V_z \in \mathfrak{I}_h^*}\psi_i(x_z, y_z)\int_{V_z}\psi_j(x, y)\mathrm{d}x\,\mathrm{d}y,$$

$$C_{ij} = \sum_{V_z \in \mathfrak{I}_h^*}\psi_i(x_z, y_z)\int_{\partial V_z}\left(\frac{D_2\partial\psi_j(x, y)}{\partial y}\mathrm{d}x - \frac{D_1\partial\psi_j(x, y)}{\partial x}\mathrm{d}y\right),$$

$$Q_{ij} = \sum_{V_z \in \mathfrak{I}_h^*}\psi_i(x_z, y_z)\int_{\partial V_z}\left(q_2\psi_j(x, y)\mathrm{d}x - q_1\psi_j(x, y)\mathrm{d}y\right).$$

If $c_0(x, y)$ is a non-zero function, then α_j^0 ($j = 1, 2, \ldots, d$) satisfy

$$\sum_{j=1}^{d}\alpha_j^0 B_{ij} = \sum_{V_z \in \mathfrak{I}_h^*}\psi_i(x_z, y_z)\int_{V_z}c_0(x, y)\mathrm{d}x\,\mathrm{d}y, \quad i = 1, 2, \ldots, d. \tag{3.23}$$

Remark 2. If $\mathfrak{I}_h$ is a uniformly regular triangulation and U_h is the space of piecewise linear function, the total number of degrees of freedom for Problem III, i.e., the number of unknown quantities is N_h (where N_h is the number of vertices of triangles in $\mathfrak{I}_h$, see [16,37]), while the number of total degrees of freedom for Problem IV is d ($d \ll l \le L \ll N$). For scientific engineering problem, the number of vertices of triangles in $\mathfrak{I}_h$ is of the order of more than tens of thousands or even exceeding a hundred million, while d is only the number of few leading eigenvalues which is chosen as the first L snapshots from the N snapshots so that it is very small (for example, in Section 5, $d = 6$, while $N_h = 5000 \times 5000 = 25 \times 10^6$). Therefore, Problem IV is a reduced-order FVE formulation based on POD method for Problem III. Moreover, since the development and change of solute content in the soil are closely related to previously given results, one may truly capture the laws of change of solute content in the soil by using existing results as snapshots to construct POD basis and by solving corresponding PDEs. Therefore, the POD methods provide a useful and important application.

4. Error estimates of solution for Problem IV and implementation of algorithm

4.1. Error estimates of solution for Problem IV

In this section, we refer to the classical FVE method to derive the error estimates of solutions for Problem IV. To this end, it is necessary to introduce some preparative lemmas. We first introduce the following discrete Gronwall Lemma (see [1,37]).

Lemma 5. *[Discrete Gronwall Lemma] If $\{a_n\}$, $\{b_n\}$, and $\{c_n\}$ are three positive sequences, and $\{c_n\}$ is monotone, that satisfy*

$$a_n + b_n \leq c_n + \bar{\lambda} \sum_{i=0}^{n-1} a_i (\bar{\lambda} > 0), \quad a_0 + b_0 \leq c_0,$$

then

$$a_n + b_n \leq c_n \exp(n\bar{\lambda}), \quad n \geq 0.$$

Noting that D_1 and D_2 are positive and bounded functions and using the same approaches as proofs in [31] or [30] yield the following two lemmas.

Lemma 6. *The bilinear form $a(c_h, \Pi_h^* w_h)$ is symmetric, bounded, and positive definite, i.e.,*

$$a(c_h, \Pi_h^* w_h) = a(w_h, \Pi_h^* c_h) = a(c_h, w_h), \quad \forall c_h, w_h \in U_h$$

and

$$a(c_h, c_h) \geq M_1 \|\nabla c_h\|_0^2, \quad a(c_h, w_h) \leq M_2 \|\nabla c_h\|_0 \|\nabla w_h\|_0, \quad \forall c_h, w_h \in U_h.$$

Lemma 7. *The following statement holds:*

$$(c_h, \Pi_h^* w_h) = (w_h, \Pi_h^* c_h), \quad \forall c_h, w_h \in U_h.$$

For any $c \in H^m(\Omega)(m = 0, 1)$ and $w_h \in U_h$,

$$|(c, w_h) - (c, \Pi_h^* w_h)| \leq Mh^{m+s} \|c\|_m \|w_h\|_n, \quad s = 0, 1.$$

Set $\|\|w_h\|\|_0 = (w_h, \Pi_h^* w_h)^{1/2}$, then $\|\cdot\|\|_0$ is equivalent to $\|\cdot\|_0$ on U_h, i.e., there exist two positive constants M_3 and M_4 such that

$$M_3 \|w_h\|_0 \leq \|\|w_h\|\|_0 \leq M_4 \|w_h\|_0, \quad \forall w_h \in U_h.$$

The following main results for Problem IV hold

Theorem 8. *Under hypotheses of Theorem 2, if $\tau \leq M_1/(4M_2^2)$, Problem IV has a unique set of solution $c_d^n \in U^d$ such that*

$$\|c_d^n\|_0^2 + \tau \sum_{i=1}^n \|\nabla c_d^i\|_0^2 \leq \frac{4\tau M_1^{-1} \exp(4n\tau M_2^2 M_1^{-1})}{\min\{M_3, M_1\}} \sum_{i=1}^n \|S_r^i\|_{-1}^2, \quad 1 \leq n \leq N. \tag{4.1}$$

And if $L^2 = O(N)$ and $k = O(h)$ is sufficiently small, then the following error estimates hold

$$\|c_h^n - c_d^n\|_0 + \tau^{\frac{1}{2}} \left(\sum_{i=1}^n \|\nabla(c_h^i - c_d^i)\|_0^2 \right)^{\frac{1}{2}} \leq M \left(\tau^{\frac{1}{2}} \sum_{j=d+1}^l \lambda_j \right)^{\frac{1}{2}}, \quad 1 \leq n \leq L. \tag{4.2}$$

Proof. Noting that $U^d \subset U_h$, for fix $\tau \leq M_1/(4M_2^2) \leq M_1/M_2^2$, we get by (2.15) and Lemmas 6 and 7 that

$$(c_d^n, \Pi_h^* c_d^n) + \tau a(c_d^n, \Pi_h^* c_d^n) - \tau b(c_h^n, \Pi_h^* c_d^n) \geq \||c_d^n\||_0^2 + M_1\tau\|\nabla c_d^n\|_0 - \tau M_2\||c_d^n\||_0\|\nabla c_d^n\|_0 \geq \||c_d^n\||_0^2$$

$$+ M_1\tau\|\nabla c_d^n\|_0 - \frac{1}{2}\||c_d^n\||_0^2 - \frac{1}{2}\tau^2 M_2^2\|\nabla c_d^n\|_0^2 \geq \alpha(\||c_d^n\||_0^2 + \tau\|\nabla c_d^n\|_0^2), \quad \forall c_d^n \in U^d, \tag{4.3}$$

where $\alpha = \min\{1/2, M_1/2\} > 0$. Thus, by Lax–Milgram Theorem (see [8,16,37]), Problem IV has a unique set of solution $c_d^n \in U^d$.

Taking $w_d = c_d^n$ in Problem IV and using (2.15), Lemmas 6 and 7, Höler inequality, and Cauchy inequality yield that

$$\||c_d^n\||_0^2 + \tau M_1\|\nabla c_d^n\|_0^2 \leq (c_d^n, \Pi_h^* c_d^n) + \tau a(c_d^n, c_d^n) = \tau(S_r^n, \Pi_h^* c_d^n) + (c_d^{n-1}, \Pi_h^* c_d^n)$$

$$+ \tau b(c_d^n, \Pi_h^* c_d^n) \leq \||c_d^n\||_0\||c_d^{n-1}\||_0 + \tau\|S_r^n\|_{-1}\|\nabla c_d^n\|_0 + M_2\tau\||c_d^n\||_0\|\nabla c_d^n\|_0 \leq \frac{1}{2}[\||c_d^n\||_0^2$$

$$+ \||c_d^{n-1}\||_0^2 + \tau M_1\|\nabla c_d^n\|_0^2] + \tau M_1^{-1}\|S_r^n\|_{-1}^2 + \tau M_2^2 M_1^{-1}\||c_d^n\||_0^2, \tag{4.4}$$

i.e.,

$$\||c_d^n\||_0^2 + \tau M_1\|\nabla \tau_d^n\|_0^2 \leq \||c_d^{n-1}\||_0^2 + 2\tau M_1^{-1}(\|S_r^n\|_{-1}^2 + M_2^2\||c_d^n\||_0^2). \tag{4.5}$$

Summing (4.5) from 1 to n yields that

$$\||c_d^n\||_0^2 + \tau M_1\sum_{i=1}^n\|\nabla c_d^i\|_0^2 \leq 2\tau M_1^{-1}\sum_{i=1}^n(\|S_r^i\|_{-1}^2 + M_2^2\||c_d^i\||_0^2), \quad 1 \leq n \leq N. \tag{4.6}$$

If τ is sufficiently small such that $\tau M_1^{-1}M_2^2 \leq 1/4$, (4.6) yields that

$$\||c_d^n\||_0^2 + \tau M_1\sum_{i=1}^n\|\nabla c_d^i\|_0^2 \leq \||c_d^n\||_0^2 + 2\tau M_1\sum_{i=1}^n\|\nabla c_d^i\|_0^2$$

$$\leq 4\tau M_1^{-1}\sum_{i=1}^n\|S_r^i\|_{-1}^2 + 4\tau M_2^2 M_1^{-1}\sum_{i=1}^{n-1}\||c_d^i\||_0^2, \quad 1 \leq n \leq N. \tag{4.7}$$

Applying Lemma 4 to (4.7) yields (4.1).

Since $U^d \subset U_h$, subtracting Problem IV from Problem III taking $w_h = w_d \in U^d$ yields that

$$(c_h^n - c_d^n, \Pi_h^* w_d) + \tau a(c_h^n - c_d^n, \Pi_h^* w_d) = \tau b(c_h^n - c_d^n, \Pi_h^* w_d) + (c_h^{n-1} - c_d^{n-1}, \Pi_h^* w_d), \quad \forall w_d \in U^d. \tag{4.8}$$

Thus, we have from (4.8), (3.17), and Lemmas 6 and 7 that

$$\||c_h^n - c_d^n\||_0^2 + \tau M_1\|\nabla(c_h^n - c_d^n)\|_0^2 \leq (c_h^n - c_d^n, \Pi_h^*(c_h^n - c_d^n)) + \tau a(c_h^n - c_d^n, c_h^n - c_d^n)$$

$$= (c_h^n - c_d^n, \Pi_h^*(c_h^n - P^d c_h^n)) + (c_h^n - c_d^n, \Pi_h^*(P^d c_h^n - c_d^n))$$

$$+ \tau a(c_h^n - P^d c_h^n, c_h^n - P^d c_h^n) + \tau a(c_h^n - c_d^n, P^d c_h^n - c_d^n) \tag{4.9}$$

$$= (c_h^n - c_d^n, \Pi_h^*(c_h^n - P^d c_h^n)) + (c_h^{n-1} - c_d^{n-1}, \Pi_h^*(P^d c_h^n - c_d^n))$$

$$+ \tau a(c_h^n - P^d c_h^n, c_h^n - P^d c_h^n) + \tau b(c_h^n - c_d^n, \Pi_h^*(P^d c_h^n - c_d^n)).$$

By (3.19) and by using Hölder inequality and Cauchy inequality, we have that

$$(c_h^n - c_d^n, \Pi_h^*(c_h^n - P^d c_h^n)) + (c_h^{n-1} - c_d^{n-1}, \Pi_h^*(P^d c_h^n - c_d^n)) \leq \||c_h^n - c_d^n\||_0\||c_h^n - P^d c_h^n\||_0$$

$$+ \||c_h^{n-1} - c_d^{n-1}\||_0\||c_h^n - P^d c_h^n\||_0 + \||c_h^{n-1} - c_d^{n-1}\||_0\||c_h^n - c_d^n\||_0 \leq Mh[\||c_h^n - c_d^n\||_0^2$$

$$+ \||c_h^{n-1} - c_d^{n-1}\||_0^2 + \|\nabla(c_h^n - P^d c_h^n)\|_0^2] + \frac{1}{2}[\||c_h^{n-1} - c_d^{n-1}\||_0^2 + \||c_h^n - c_d^n\||_0^2], \tag{4.10}$$

$$\tau b(c_h^n - c_d^n, \Pi_h^*(P^d c_h^n - c_d^n)) + \tau a(c_h^n - P^d c_h^n, c_h^n - P^d c_h^n) \le M\tau[\|\|c_h^n - c_d^n\|\|_0^2$$

$$+ \|\nabla(c_h^n - P^d c_h^n)\|_0^2] + \frac{\tau M_1}{2}\|\nabla(c_h^n - c_d^n)\|_0^2. \tag{4.11}$$

If $k = O(h)$, inputting (4.10) and (4.11) into (4.9) and reducing it yield that

$$\|\|c_h^n - c_d^n\|\|_0^2 + \tau M_1\|\nabla(c_h^n - c_d^n)\|_0^2 \le M\tau[\|\|c_h^n - c_d^n\|\|_0^2 + \|\|c_h^{n-1} - c_d^{n-1}\|\|_0^2$$

$$+ \|\nabla(c_h^n - P^d c_h^n)\|_0^2] + \|\|c_h^{n-1} - c_d^{n-1}\|\|_0^2. \tag{4.12}$$

Summing (4.12) from 1 to n yields that

$$\|\|c_h^n - c_d^n\|\|_0^2 + M_1\tau\sum_{i=1}^{n}\|\nabla(c_h^i - c_d^i)\|_0^2 \le M\tau\sum_{i=0}^{n}\|\|c_h^i - c_d^i\|\|_0^2 + M\tau\sum_{i=1}^{n}\|\nabla(c_h^i - P^d c_h^i)\|_0^2. \tag{4.13}$$

If τ is sufficiently small such that $\tau M \le 1/2$, we have from (4.13) and Lemma 7 that

$$\|c_h^n - c_d^n\|_0^2 + \tau\sum_{i=1}^{n}\|\nabla(c_h^i - c_d^i)\|_0^2 \le M\tau\sum_{i=0}^{n-1}\|\|c_h^i - c_d^i\|\|_0^2 + M\tau\sum_{i=1}^{n}\|\nabla(c_h^i - P^d c_h^i)\|_0^2. \tag{4.14}$$

If $L^2 = O(N)$, applying Lemmas 4 and 5 to (4.14) yields that

$$\|c_h^n - c_d^n\|_0^2 + \tau\sum_{i=1}^{n}\|\nabla(c_h^i - c_d^i)\|_0^2 \le M\tau\exp(M\tau n)\sum_{i=1}^{n}\|\nabla(c_h^i - P^d c_h^i)\|_0^2$$

$$\le M\tau\sum_{i=1}^{n}\|\nabla(c_h^i - P^d c_h^i)\|_0^2 \le M\tau^{\frac{1}{2}}\sum_{j=d+1}^{l}\lambda_j, \quad 1 \le n \le L. \tag{4.15}$$

Applying triangle inequality $\sqrt{a^2 + b^2} \ge \sqrt{(a^2 + b^2 + 2ab)/2} = (a + b)/\sqrt{2}(a \ge 0, b \ge 0)$ to (4.15) yields (4.2) which completes the proof of Theorem 8. □

Combining Theorem 2 with 8 and using again the triangular inequality $\sqrt{a^2 + b^2} \ge (a + b)/\sqrt{2}(a \ge 0, b \ge 0)$ yields the following result.

Theorem 9. *Under hypotheses of Theorem 8, the error estimates between the solutions for Problem* II *and the solutions for the reduced-order Problem* IV *are*

$$\|c(t_n) - c_d^n\|_0 + \tau^{\frac{1}{2}}\left(\sum_{i=1}^{n}\|\nabla(c(t_i) - c_d^i)\|_0^2\right)^{\frac{1}{2}} \le M\left[h^2 + \tau + \left(\sum_{j=d+1}^{l}\lambda_j\right)^{1/2}\right], \quad 1 \le n \le L. \tag{4.16}$$

Remark 3. The inequality (4.1) in Theorem 8 shows that the solutions $c_d^n(n = 1, 2, \ldots, N)$ to Problem VI are stable and continuously dependent on source term $S_r(x, y, t)$ (and initial value function $c_0(x, y)$ if $c_0(x, y)$ is a nonzero function). The condition $L^2 = O(N)$ in Theorem 8 shows the relationship between the number L of snapshots and the number N of all time instances. Therefore, it is unnecessary to take the total number of transient solutions at all time instances t_n as snapshots (see [26,27]). Theorems 8 and 9 have, respectively, provided the error estimates between the solution of the reduced-order FVE formulation Problem IV and the solution of classical FVE formulation Problem III and Problem II, which can guide us in choosing the number d of POD bases.

4.2. Implementation of extrapolation algorithm for Problem IV

In the following, we provide the implementation of extrapolation algorithm for solving Problem IV which consists of the following seven steps.

Step 1. Generate the snapshots ensemble

$$W_i(x, z) = c_h^i, \quad i = 1, 2, \ldots, L \ll N,$$

which may be the solutions for Problem III, physical system trajectories by drawing samples from experiments and interpolation (or data assimilation), or previous given results;

Step 2. Generate the correlation matrix $A = (A_{ik})_{L \times L}$, where $A_{ik} = (W_i, W_k)_U / L$, $(W_i, W_k)_U = (\nabla c_h^i, \nabla c_h^k)$, and $(\cdot, \cdot)$ is L^2-inner product;

Step 3. Solving the eigenvalue problem

$$A\boldsymbol{v} = \lambda \boldsymbol{v}, \quad \boldsymbol{v} = (a_1, a_2, \ldots, a_L)^T$$

obtains positive eigenvalues λ_k and the associated eigenvectors $\boldsymbol{v}^k = (a_1^k, a_2^k, \ldots, a_L^k)$ $(k = 1, 2, \ldots, l = dim\{W_1, W_2, \ldots, W_L\})$;

Step 4. For a given error δ needed, decide on the number d of POD bases such that $\tau + h^2 + \left(\tau^{1/2} \sum_{j=d+1}^{l} \lambda_j \right)^{1/2} \leq \delta$;

Step 5. Generate POD basis $\psi_k(x, y)$:

$$\psi_k(x, y) = \frac{1}{\sqrt{L\lambda_k}} \sum_{i=1}^{L} a_i^k w_i(x, y) = \frac{1}{\sqrt{L\lambda_k}} \sum_{i=1}^{L} a_i^k c_h^i, k = 1, 2, \ldots, d.$$

Step 6. Solving the following system of equations which is only comprised of d degrees of freedom

$$\sum_{j=1}^{d} \alpha_j^0 B_{ij} = \sum_{V_z \in \mathfrak{I}_h^*} \psi_i(x_z, y_z) \int_{V_z} c_0(x, y) \mathrm{d}x \, \mathrm{d}y, \quad i = 1, 2, \ldots, d;$$

$$\sum_{j=1}^{d} \alpha_j^n [B_{ij} + \tau C_{ij} + \tau Q_{ij}] = F_i^n + \sum_{j=1}^{d} \alpha_j^{n-1} B_{ij}, \qquad i = 1, 2, \ldots, d, \quad n = 1, 2, \ldots, N,$$

where

$$B_{ij} = \sum_{V_z \in \mathfrak{I}_h^*} \psi_i(x_z, y_z) \int_{V_z} \psi_j(x, y) \mathrm{d}x \, \mathrm{d}y,$$

$$C_{ij} = \sum_{V_z \in \mathfrak{I}_h^*} \psi_i(x_z, y_z) \int_{\partial V_z} \left(\frac{D_2 \partial \psi_j(x, y)}{\partial y} \mathrm{d}x - \frac{D_1 \partial \psi_j(x, y)}{\partial x} \mathrm{d}y \right),$$

Table 1
Parameters of the solute transport problems (s denotes second).

$D_1 = D_2$	$q_1 = q_2$	$\overline{\Omega}$	τ	$\triangle x = \triangle y$	T
0.01 cm^2/s	0.8 cm/s	$0 \le x, y \le 50$ cm	0.02 s	0.01 cm	4 s

$$Q_{ij} = \sum_{V_z \in \mathfrak{I}_h^*} \psi_i(x_z, y_z) \int_{\partial V_z} \left(q_2 \psi_j(x, y) \mathrm{d}x - q_1 \psi_j(x, y) \mathrm{d}y \right),$$

$$F_i^n = \sum_{V_z \in \mathfrak{I}_h^*} \psi_i(x_z, y_z) \int_{V_z} S_r(x, y, t_n) \mathrm{d}x \, \mathrm{d}y$$

obtains $(\alpha_1^n, \alpha_2^n, \ldots, \alpha_d^n)^T \in \mathbb{R}^d$ $(n = 1, 2, \ldots, L, L+1, \ldots, N)$ further yields the solutions $c_d^n = \alpha_1^n \psi_1 + \alpha_2^n \psi_2 + \cdots + \alpha_d^n \psi_d$ $(n = 1, 2, \ldots, L, L+1, \ldots, N)$.

Step 7. If $\|c_d^{n-1} - c_d^n\|_0 \ge \|c_d^n - c_d^{n+1}\|_0$ $(n = L, L+1, \ldots, N-1)$, c_d^n $(n = 1, 2, \ldots, N)$ are the solutions for Problem IV whose errors are more than $\tau + h^2 + \left(\tau^{1/2} \sum_{j=d+1}^l \lambda_j \right)^{1/2}$. Else, i.e., if $\|c_d^{n-1} - c_d^n\|_0 < \|c_d^n - c_d^{n+1}\|_0$ $(n = L, L+1, \ldots, N-1)$, let $W_i = c_d^i$ $(i = n - L - 1, n - L - 2, \ldots, n)$, repeat **Step 1** to **Step 6**.

5. A numerical experiment

In this section, a numerical experiment using the two-dimensional solute transport model is conducted in order to validate the feasibility and efficiency of the reduced-order FVE formulation based on the POD method.

For the sake of convenience, without loss of generality, herein we consider a simple two-dimensional solute transport model as an example, whose approach could be directly applied to numerical computations for two-dimensional solute transport models with real-life application, which can be described as follows.

Find $c(x, y, t)$ such that, for any $T > 0$,

$$\begin{cases} \dfrac{\partial c}{\partial t} + q_1 \dfrac{\partial c}{\partial x} + q_2 \dfrac{\partial c}{\partial y} - \dfrac{\partial}{\partial x} \left(D_1 \dfrac{\partial c}{\partial x} \right) - \dfrac{\partial}{\partial y} \left(D_2 \dfrac{\partial c}{\partial y} \right) = S_r, & (x, y) \in \Omega, \quad t \in (0, T), \\ c(x, y, 0) = c_0(x, y), & (x, y) \in \Omega, \\ c(x, y, t) = c_\Gamma(x, y, t), & (x, y) \in \Gamma, \quad t \in (0, T), \end{cases} \tag{5.1}$$

where Γ is the boundary of the domain $\Omega = (0, 50) \times (0, 50)$ cm^2, $c_\Gamma(x, y, t)$ denotes the solute density on Γ. Without loss of generality, we might as well take $S_r = 0$, then the two-dimensional solute transport equations and the initial condition can be written as follows.

$$\begin{cases} \dfrac{\partial c}{\partial t} + q_1 \dfrac{\partial c}{\partial x} + q_2 \dfrac{\partial c}{\partial y} - \dfrac{\partial}{\partial x} \left(D_1 \dfrac{\partial c}{\partial x} \right) - \dfrac{\partial}{\partial y} \left(D_2 \dfrac{\partial c}{\partial y} \right) = 0, & (x, y) \in \Omega, \quad t \in (0, T), \\ c(x, y, 0) = \begin{cases} 0.5, & y = x = 0, \\ 0, & \text{others}, \end{cases} \\ c(0, 0, t) = 0.5, t \in (0, T) \\ c_\Gamma(x, y, t) = c(x, y, 0). \end{cases} \tag{5.2}$$

In numerical simulation, we employ the parameters listed in Table 1.

We first divide the field $\overline{\Omega}$ into 5000×5000 small squares with side length $\triangle x = \triangle y = 0.01$, and then link the diagonal of the square to divide each square into two triangles in the same direction, which constitutes a triangularization $\mathfrak{I}_h$. Thus $h = \sqrt{2} \times 0.01$. In order to satisfy $\tau = O(h)$, we take time step size as $\tau = 0.02$. The dual decomposition $\mathfrak{I}_h^*$ is taken as the barycenter dual decomposition, i.e., the barycenter of the right triangle $K \in \mathfrak{I}_h$ is taken as the node of the dual partition.
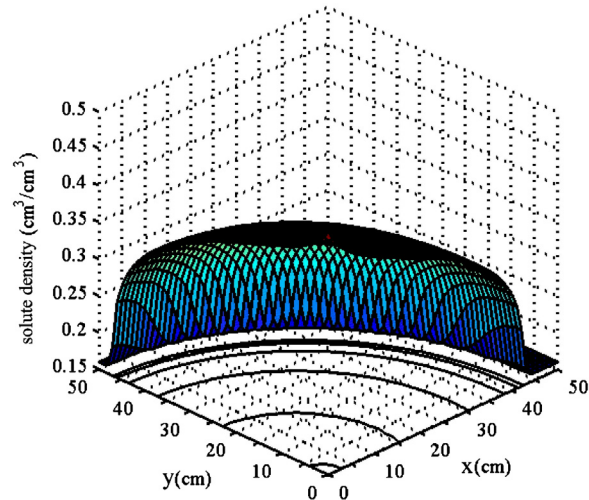
Fig. 2. FVE solution figure when $t = 200\tau$.

We first find a group of numerical solutions c_h^n of classical FVE method (i.e., Problem III) when $n = 1, 2, \ldots, 20$, i.e., at time $t = 1\tau, 2\tau, \ldots, 20\tau$, constructing 20 numerical solutions which are taken as 20 snapshots. And then, we find 20 eigenvalues which are arranged in a non-increasing order, and 20 eigenvectors corresponding to the twenty eigenvalues and using (3.13) and (3.14) we construct a group of POD bases. Take the first 6 POD bases from 20 POD bases to expand into subspace U^d and find a numerical solution at $t = 200\tau$ with Problem IV according to the seven steps of Section 4.2, which is still convergent without refreshing the POD basis, we obtain the numerical solution depicted graphically in Figs. 3 and 5, respectively. The classical FVE solution of Eq. (5.2) at $t = 200\tau$ is depicted graphically in Figs. 2 and 4, respectively. Every two images in Figs. 2 and 3, as well Figs. 4 and 5 are exhibiting a quasi-identical similarity, respectively.

When we take 6 POD bases and $\tau = 0.02$, by computing we obtain that $[\tau^{1/2} \sum_{j=7}^{20} \lambda_j]^{1/2} \leq 0.04$. Fig. 6 computationally shows the errors between the solutions c_d^n of Problem IV with 20 different numbers of POD bases and a set of solutions c_h^n of classical FVE formulation Problem III at $t = 200\tau$ (i.e., $n = 200$), respectively. Comparing the classical FVE formulation Problem III with the reduced-order FVE formulation Problem IV containing 6 POD bases
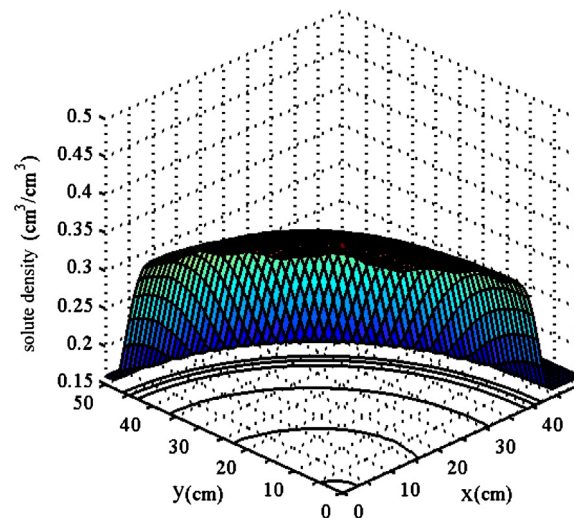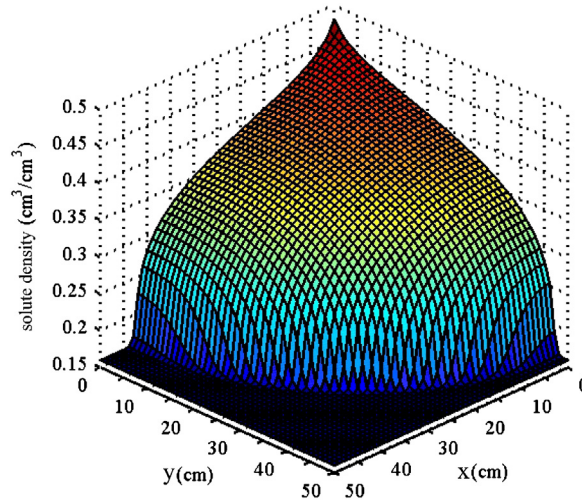

Fig. 3. POD solution figure when $t = 200\tau$.

Fig. 4. The result of rotating Fig. 2 by 180°.

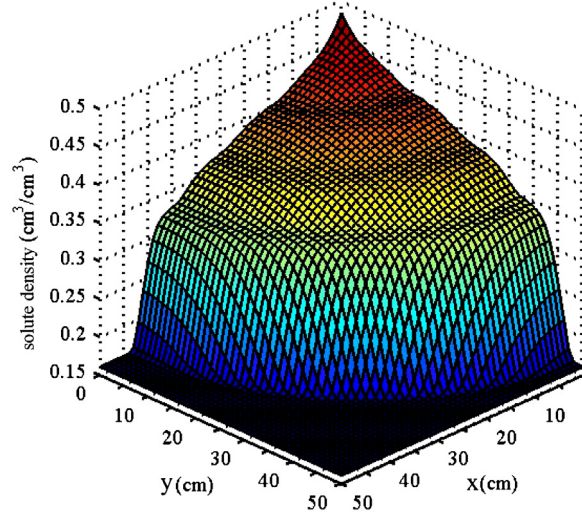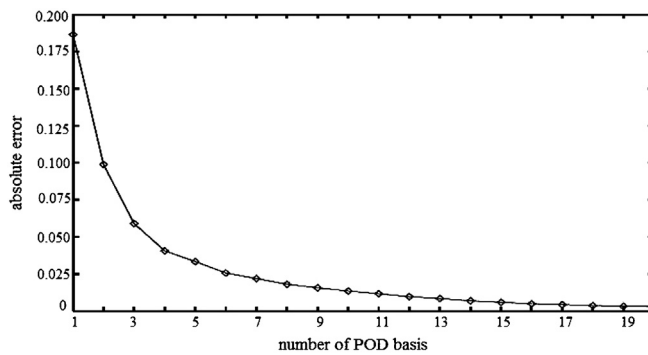Fig. 5. The result of rotating Fig. 3 by 180°.

Fig. 6. When $t = 200\tau$, the errors between solutions of Problem IV with different number of POD bases for a group of 20 snapshots and the classical FVE formulation Problem III with piecewise 1-th degree polynomials.

implementing the numerical simulation computations when time $t = 200\tau$, we find that for the classical FVE formulation Problem III with piecewise linear polynomials for c_h^n, which has $5000 \times 5000 = 25 \times 10^6$ degrees of freedom, the required computing time is 18 minutes, while for the reduced-order FVE formulation Problem IV with 6 POD bases, which has only 6 degrees of freedom, the corresponding time is only six seconds, i.e., the required computing time to solve the classical FVE formulation Problem III is by a factor of 180 times larger than that required for the reduced-order FVE formulation Problem IV with 6 POD bases, while the errors between their respective solutions do not exceed 0.04. Though our examples are in some sense a recomputation of what we have already computed by classical FVE formulation at the first 20 steps, when we compute actual problems, we may construct the snapshots and POD basis with interpolation or data assimilation by drawing samples from experiments, then solve directly the reduced-order FVE formulation. Thus it is unnecessary to solve classical FVE formulation, meaning that the computational load could be alleviated and CPU requirements in the computational process are considerably saved. It is also shown that finding the approximate solutions for two-dimensional solute transport problems with the reduced-order FVE formulation Problem IV is computationally very effective. Moreover, the results for numerical examples are consistent with those obtained for the theoretical case.

6. Conclusions and perspectives

In this paper, we have employed the POD method to establish a reduced-order FVE formulation for two-dimensional solute transport problems with real practical use. We have analyzed the errors between the solutions of the classical FVE formulation and solutions of the reduced-order FVE formulation based on the POD method. We also provided the implementation of extrapolation algorithm for solving the reduced-order FVE formulation, i.e., Problem IV, and supplied a reduced-order modelling and the implementation of algorithm for solving reduced-order FVE formulation. This has shown that our present method constitutes an improvement and innovation of the existing methods (e.g., see [13,36,3,51]). The existing methods (e.g., see [13,36,3,51]) utilize the given numerical solutions at all time nodal points to construct the snapshots and POD basis, then recompute the POD numerical solutions at the same all time nodal points (without using extrapolation); however, in the present paper, we only use the first few given numerical solutions obtained from classical FVE formulation (which are also obtained by drawing samples from experiments) to construct the snapshots and POD basis and establish the reduced-order FVE formulation based on POD technique. Then in order to find the solutions for the rest of the time nodal points we use extrapolation algorithm, thus, we do not only provide a new theoretical basis and computing way for practical applications, but also exploit efficiently the important role of POD method to forecast future cases with given data.

Concerning the theoretical error, the error estimate has been verified to provide quite good results, namely both the theoretical error and the computing errors coincide within plot accuracy, thus validating both the feasibility and efficiency of our reduced-order FVE formulation. Though snapshots and POD basis of our numerical examples are constructed with the solution of the classical FVE formulation at the first 20 steps, when one computes actual two-dimensional solute transport problems, this process can be omitted in actual applications and one may construct the snapshots and POD basis using interpolation or data assimilation by drawing samples from experiments, then solve Problem IV, while it is unnecessary to solve Problem III, such that the computational load requirement could be alleviated and a large amount of CPU time required in the computational process can be saved. Therefore, the method presented in this paper holds a good prospect for extensive applications. Future research work in this area will aim at extending the reduced-order FVE formulation, applying it to realistic solute transport problems, operational forecast system and to a set of more complicated PDEs such as the atmosphere quality forecast system and the ocean fluid forecast system.

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