

FINITE VOLUME ELEMENT METHOD FOR THE STOCHASTIC ADVECTIVE-DISPERSIVE EQUATION IN POROUS MEDIA

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ABSTRACT. In this paper, an advective-dispersive contaminant transport model with a chemical reaction is considered. A quadratic finite volume element method (QFVEM) is presented for the numerical solution of contaminant transport model. In addition, the advective-dispersive contaminant transport equation in the presence of Gaussian white noise is considered. Time stochasticity as a source term, spatial stochasticity as a source term, and time stochasticity in the boundary conditions will be treated respectively. Monte Carlo method will be used in random space and quadratic finite volume element method will be used in physical space. Numerical results demonstrate that the effect of stochasticity of the boundaries is relatively less important than the effect of distributed-source stochasticity on the concentration.

AMS (MOS) Subject Classification. 39A10, 65C20.

1. INTRODUCTION

Practical problems [7], such as, groundwater management, groundwater pollution control, and aquifer restoration require the use of a mathematical model to predict the spatial distribution and time evolution of a contaminant plume in a system of aquifers responding to a particular source. The good example is the advective-dispersive equation, which still is the heart of dispersion model in porous media. The governing equation for contaminant transport through homogeneous porous media is given by (Freeze and Cherry 1979):

$$(1.1) \quad \frac{\partial C}{\partial t} = -v \frac{\partial C}{\partial x} + D \frac{\partial^2 C}{\partial x^2} - \lambda C$$

where C is the contaminant concentration (mg/l), t the time (day), v the velocity of flow (m/day), x the distance along the direction of flow upstream boundary of the modeled domain (m), D the dispersion coefficient (m^2/day), and λ the first-order reaction rate constant or decay rate constant (day^{-1}). The following initial and

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boundary conditions are considered:

$$C(x, 0) = f(x), \quad C(0, t) = k(t), \quad C(\infty, t) = 0 \text{ or } \frac{\partial C(\infty, t)}{\partial x} = 0,$$

here $f(x)$ is the initial concentration distribution across the aquifer, $k(t)$ is a time-dependent concentration at the origin.

The finite volume element method (FVEM) is a well-known numerical method especially in the hydrodynamics field. The method has been introduced and analyzed by Li and his collaborators since 1980s [12]. The FVEM uses a volume integral formulation of the original problem and a finite element partition of the domain to discretize the equations. The approximate solution is chosen from a finite element space [4, 3, 12]. Based on the weak form of the considered problem, this method has its own advantages: reasonable accuracy, conservation of physical quantity locally and high efficiency, which make it be applied widely in computation fluid dynamics [27, 26, 25, 6, 11, 31, 32]. We will use it for our following simulations when noise is added in.

In addition, the convection-dominated diffusion problem has strongly hyperbolic characteristics, therefore constructing a numerical method to solve such a problem is difficult. When use central difference method, although it has second-order accuracy, it produces numerical diffusion and oscillation near discontinuity. Douglas and Russell used the character finite element method and character finite difference method [5] to overcome the difficulties. Tabata and his collaborators have been studying upwind schemes for the convection-diffusion problem since 1977 [1, 22, 23]. Yuan presented an upwind finite difference fractional step method [29] and a character finite element alternating direction method [30] for simulation in high-dimensional situation. Many other techniques have been proposed to overcome the method instability in order to improve the solution accuracy [8, 10, 16, 21].

With the above consideration, we mainly provide a quadratic finite volume element method (QFVEM) due to the ease of implementation. The efficiency and convergence order of the method are investigated. We achieve balance between obtaining reliable control of the error and efficient use of the available computational resources. There are various approaches in deriving finite volume element approximations of advective-dispersive equation (see, for instance [13, 15, 17, 24]).

So far, most attention was paid to the advective-dispersive equation with or without reaction in homogeneous porous media, ignoring the effects from the circumstances. We know that the solution of the advective-dispersive equation in porous media is subject to very special circumstances. It is necessary for a method capable of solving this equation and predicting the time and space evolution of the contaminant migration in aquifers subject to any size or any form of stochasticity. The objective of the present paper is to study different sources of stochasticity affecting the process

of mass transport and their individual effects on the behaviour of the output concentration of the system. We use a well-known stochastic process in the examples, namely the white Gaussian process [9, 28]. We do so for simplicity and because the properties of this process closely resemble many physically-realizable processes after the deterministic trend has been removed.

The general stochastic advective-diffusion equation [18, 19, 20] in porous media may be treated as a stochastic evolution equation of the form

$$(1.2a) \quad \frac{\partial C}{\partial t} - D \frac{\partial^2 C}{\partial x^2} + v \frac{\partial C}{\partial x} + \lambda C = g(x, t, \omega),$$

$$(1.2b) \quad C(0, t) = k(t, \omega), \quad C(\infty, t) = 0, \quad C(x, 0) = f(x),$$

where $g(x, t, \omega)$ represents a stochastic source or sink disturbing the system, $k(t, \omega)$ is the time-dependent concentration process at the origin.

In this paper, we will employ Monte Carlo method [9, 27, 14, 28] for discretization in random space and QFVEM [12, 31, 32] for discretization in physical space. The advantage of Monte Carlo method is clear, i.e., ease of implementation for complex problems, which makes it popular in stochastic computations. We shall illustrate the application of the above methods to the solution of the advective-dispersive equation in porous media subject to either time stochasticity as a source term, spatial stochasticity as a source term, and time stochasticity in the boundary conditions. The primary objective of the current work is to study the influence of a noise term on the evolution of concentration.

The article is organized as follows. Our numerical method is described in section 2, which will give numerical results for deterministic problems. In section 3, we present numerical results for the stochastic advective-dispersive equation with different cases of stochasticity. The conclusions are summarized in the last section.

2. NUMERICAL METHOD

Consider Eq. (1.1) in the interval $[0, l]$, let $C \in C^1[0, l] \cap C^2(0, l)$ be the solution of Eq. (1.1), and $H_E^1[0, l] = \{w \in H^1[0, l] : w(l) = 0\}$. Use any function $w \in H_E^1[0, l]$ (called a test function) to multiply (1.1) and integrate it on $[0, l]$ using integration by parts, then apply the boundary conditions, we obtain the variational problem related to (1.1) is: Find $C = C(\cdot, t) \in H^1[0, l]$, $(0 \leq t \leq T)$ such that

$$(2.1) \quad \left(\frac{\partial C}{\partial t}, w \right) + A(C, w) = (f, w),$$

where $f = \lambda C$, (\cdot, \cdot) denotes the inner product of $L^2([0, l])$ and $A(C, w) = \int_0^l \left(D \frac{\partial C}{\partial x} \frac{\partial w}{\partial x} + v \frac{\partial C}{\partial x} w \right) dx$.

2.1. Finite volume element schemes. The region $[0, l]$ can be decomposed into a grid T_h with a set of evenly spaced nodes

$$0 = x_0 < x_1 < x_2 < \cdots < x_{N-1} < x_N = l.$$

Denote $T_h = \{I_i : I_i = [x_{i-1}, x_i], i = 1, 2, \dots, N\}$, $h = x_i - x_{i-1}$. To obtain quadratic basis functions, we use the midpoints $x_{i-1/2} = (x_i + x_{i-1})/2$ of the element I_i as the interpolation points. Accordingly we place a dual grid T_h^* with nodes

$$0 = x_0 < x_{1/4} < x_{3/4} < \cdots < x_{N-3/4} < x_{N-1/4} < x_N = l,$$

where $x_{i-k/4} = x_i - \frac{k}{4}h$, ($k = 1, 3; i = 1, 2, \dots, N$). Then the dual elements are constituted by two groups: $T_h^* = \{I_{i-1/2}^* : I_{i-1/2}^* = [x_{i-3/4}, x_{i-1/4}], i = 1, 2, \dots, N\} \cup \{I_i^* : I_i^* = [x_{i-1/4}, x_{i+1/4}], i = 1, 2, \dots, N-1, I_0^* = [x_0, x_{1/4}], I_N^* = [x_{N-1/4}, x_N]\}$.

Select trial function space C_h as the quadratic element space of Lagrange type with respect to T_h . The basis functions with respect to the nodes x_i and $x_{i-1/2}$ are as follows:

$$\phi_i(x) = \begin{cases} (2\frac{|x-x_i|}{h} - 1)(\frac{|x-x_i|}{h} - 1), & x_{i-1} \leq x \leq x_{i+1}, \\ 0, & \text{elsewhere,} \end{cases}$$

$$\phi_{i-1/2}(x) = \begin{cases} 4(1 - \frac{x-x_{i-1}}{h})\frac{x-x_{i-1}}{h}, & x_{i-1} \leq x \leq x_i, \\ 0, & \text{elsewhere.} \end{cases}$$

Then the numerical solution c_h for Eq. (1.1) can be uniquely written as

$$(2.2) \quad c_h = \sum_{i=1}^N [u_i \phi_i(x) + u_{i-1/2} \phi_{i-1/2}(x)],$$

where $c_i = c_h(x_i, t)$, $c_{i-1/2} = c_h(x_{i-1/2}, t)$. So in the element I_i , we have

$$c_h = c_{i-1}(2\mu - 1)(\mu - 1) + 4c_{i-1/2}\mu(1 - \mu) + c_i(2\mu - 1)\mu,$$

$$\dot{c}_h = c_{i-1}(4\mu - 3)/h + c_{i-1/2}(-8\mu + 4)/h + c_i(4\mu - 1)/h,$$

where $\mu = (x - x_{i-1})/h$.

The test function space W_h corresponding to T_h^* is taken as the piecewise constant function space. The test functions of the nodes x_j and $x_{j-1/2}$ are

$$\psi_j(x) = \begin{cases} 1, & x_{j-1/4} \leq x \leq x_{j+1/4}, \\ 0, & \text{elsewhere,} \end{cases}$$

$$\psi_{j-1/2}(x) = \begin{cases} 1, & x_{j-3/4} \leq x \leq x_{j-1/4}, \\ 0, & \text{elsewhere.} \end{cases}$$

Any $w_h \in W_h$ can be uniquely expressed as

$$w_h = \sum_{j=1}^N [w_j \psi_j(x) + w_{j-1/2} \psi_{j-1/2}(x)],$$

where $w_j = w_h(x_j, t)$, $w_{j-1/2} = w_h(x_{j-1/2}, t)$.

Corresponding to the above chosen subspaces C_h and W_h , substituting (2.2) into (2.1), and using the backward Euler scheme to discretize the time derivation, we obtain the following fully-discrete QFVEM scheme:

$$\left(\frac{c_h^{n+1} - c_h^n}{\Delta t}, w_h \right) + A(c_h^{n+1}, w_h) = (f(c_h^{n+1}), w_h), \quad \forall w_h \in W_h,$$

which can also be written as

$$(2.3) \quad \begin{cases} \frac{h}{2\Delta t}(c_j^{n+1} - c_j^n) = \frac{2D}{h}(c_{j+1/2}^{n+1} - 2c_j^{n+1} + c_{j-1/2}^{n+1}) - \\ v \left(\frac{1}{8}c_{j-1}^{n+1} - \frac{3}{4}c_{j-1/2}^{n+1} + \frac{3}{4}c_{j+1/2}^{n+1} - \frac{1}{8}c_{j+1}^{n+1} \right) - \frac{\lambda h}{2}c_j^{n+1}, \\ j = 1, 2, \dots, N-1, \\ \frac{h}{2\Delta t}(c_{j-1/2}^{n+1} - c_{j-1/2}^n) = \frac{2D}{h}(c_j^{n+1} - 2c_{j-1/2}^{n+1} + c_{j-1}^{n+1}) - \\ v \left(\frac{1}{2}c_j^{n+1} - \frac{1}{2}c_{j-1}^{n+1} \right) - \frac{\lambda h}{2}c_{j-1/2}^{n+1}, j = 1, 2, \dots, N, \end{cases}$$

where Δt is time step size, $c_j^n = c_j(n\Delta t)$.

2.2. Numerical experiments. In this section, we validate the QFVEM schemes on the deterministic problem. Now we define the following error norms:

$$L_\infty = \max |C_i^n - (c_h)_i^n|, \quad L_2 = \sqrt{\sum_{i=1}^N (C_i^n - (c_h)_i^n)^2 h}.$$

The convergence rate is computed by applying the formula

$$(2.4) \quad r = \frac{1}{\ln(2)} \ln \left(\frac{\|c_{2h,j} - C_j\|}{\|c_{h,j} - C_j\|} \right),$$

where c_{2h} is the numerical solution with space step size $2h$, C is the analytic solution, and N is the number of nodes.

Consider the following initial-boundary value problem

$$(2.5a) \quad \frac{\partial C}{\partial t} = \frac{\partial C}{\partial x} + 0.001 \frac{\partial^2 C}{\partial x^2} + 0.001C, \quad (x, t) \in [0, 2\pi] \times [0, T],$$

$$(2.5b) \quad C(x, 0) = \sin x, \quad C(0, t) = \sin t, \quad C(2\pi, t) = \sin(2\pi + t).$$

The exact solution of (2.5) is $C(x, t) = \sin(x+t)$. Using the method presented above, we can obtain the QFVEM schemes of (2.5). The problem is solved at $T = 5$.

The L_2 and L_∞ error norms are displayed in Table 1 with $\frac{\Delta t}{h^2} = 1$. Examination of the table shows that the error measures of the finite volume element schemes diminish quadratically as the space step size becomes halved and time step size becomes a quarter, which is consistent with the use of quadratic element space of Lagrange type. We compare the relative error between QFVEM and finite difference method

(FDM) in Fig. 1 and Fig. 2, it is much obvious that QFVEM is more accurate than FDM.

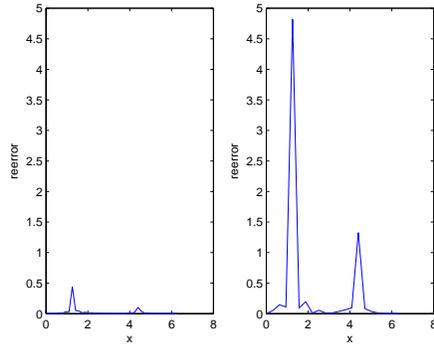


FIGURE 1. Comparison of relative error between QFVEM (left) and FDM (right) at $T=5$ with $N=20$ and $\Delta T = \frac{1}{1000}$.

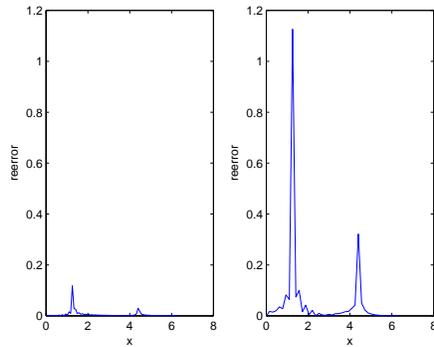


FIGURE 2. Comparison of relative error between QFVEM (left) and FDM (right) at $T=5$ with $N=40$ and $\Delta T = \frac{1}{1000}$.

TABLE 1. Error norms of numerical solution at various resolutions using FVEM.

h	L_∞ error	r	L_2 error	r
$\frac{2\pi}{40}$	9.1907e-002		7.9084e-002	
$\frac{2\pi}{80}$	2.0593e-002	2.16	1.7452e-002	2.18
$\frac{2\pi}{160}$	4.7574e-003	2.00	4.3135e-003	2.03
$\frac{2\pi}{320}$	1.1370e-003	2.06	1.0887e-003	1.99
$\frac{2\pi}{640}$	2.6093e-004	2.12	2.7257e-004	2.00

3. NUMERICAL SIMULATION OF THE STOCHASTIC ADVECTIVE-DISPERSIVE EQUATION

In this section we present some numerical results on evolution of concentration in the presence of noise. We will perform Monte Carlo simulation to obtain some significant statistical information. In Monte Carlo method [9, 14, 28], we need generate realizations of random inputs based on a prescribed probability distribution. For each realization the data are fixed and the problem becomes deterministic. Upon solving the deterministic equations with one realization, we can collect an ensemble of solutions. From this ensemble the influence of noise on the concentration will be numerically investigated.

3.1. Case 1: A distributed source problem. Time stochasticity. The advective-dispersive equation with stochastic force may be used to model the effect of unknown environment quantities affecting the concentration distribution, errors in the estimate of parameter values, errors generated in the development of the model, and uncertain chemical reactions between the fluid and the porous matrix.

In this section, we study the kind of problems when a time-stochastic distributed source dominates the uncertainty of the system. We consider that the random function g in Eq. (1.2) is a white Gaussian noise process in time and smooth in space, the boundary condition $k(t)$ is a constant source function C_0 . Eq. (1.2) becomes

$$(3.1a) \quad \frac{\partial C}{\partial t} - D \frac{\partial^2 C}{\partial x^2} + v \frac{\partial C}{\partial x} + \lambda C = \frac{dB(t)}{dt},$$

$$(3.1b) \quad C(0, t) = C_0, C(\infty, t) = 0, C(x, 0) = 0,$$

where $\frac{dB(t)}{dt} = \omega$ is a white Gaussian process with mean zero δ -correlated:

$$(3.2) \quad \langle \omega(t) \rangle = 0, \langle \omega(t_1) \omega(t_2) \rangle = q \delta(t_2 - t_1),$$

here $\langle \cdot \rangle$ means average, q is the variance parameter and B represents Brownian motion or Winner process [9, 28]. The solution to Eq. (3.1) is now considered to be a random variable. Eq. (3.1) is called a stochastic partial differential equation, with $C(x, t, \omega)$ now depending on a random noise term. The finite volume element schemes of (3.1)

become:

$$\left\{ \begin{array}{l} \frac{h}{2\Delta t}(c_j^{n+1} - c_j^n) - \frac{2D}{h}(c_{j+1/2}^{n+1} - 2c_j^{n+1} + c_{j-1/2}^{n+1}) + \\ v \left(\frac{1}{8}c_{j-1}^{n+1} - \frac{3}{4}c_{j-1/2}^{n+1} + \frac{3}{4}c_{j+1/2}^{n+1} - \frac{1}{8}c_{j+1}^{n+1} \right) + \frac{\lambda h}{2}c_j^{n+1} = \\ \frac{h}{2\Delta t}(B_j^{n+1} - B_j^n), j = 1, 2, \dots, N-1, \\ \frac{h}{2\Delta t}(c_{j-1/2}^{n+1} - c_{j-1/2}^n) - \frac{2D}{h}(c_j^{n+1} - 2c_{j-1/2}^{n+1} + c_{j-1}^{n+1}) + \\ v \left(\frac{1}{2}c_j^{n+1} - \frac{1}{2}c_{j-1}^{n+1} \right) + \frac{\lambda h}{2}c_{j-1/2}^{n+1} = \frac{h}{2\Delta t}(B_{j-1/2}^{n+1} - B_{j-1/2}^n), \\ j = 1, 2, \dots, N. \end{array} \right.$$

We are interested in seeing how the FVEM scheme compares to the deterministic solution when noise is introduced and the ensemble average is computed. An average pore velocity $v = 0.2$ (m/day), a dispersion coefficient $D = 0.01$ (m^2/day), a concentration at the original $C_0 = 10.0$ (mg/l), and a reaction rate constant $\lambda = 0.01$ are assumed. The value of q is entirely arbitrary here. We take $N = 80$ and $\Delta t = h^2$ in our simulation. Each of these runs is done over the space interval $[0, 40]$, where a run is defined as one realization of the solution, these solutions are then averaged over 400 runs. Fig. 3 shows the stochastic concentration at $x = 5$ (m) from 200 runs to 500 runs. Obviously, there is no significant differences between the results of different runs. Consider the cost of time, we will choose runs=500 in the following.

Fig. 4 is a plotter output of the program for points in space $x = 2.5$ (m) and $x = 5$ (m) from the original with $q = 0.05$, the solid line represents the evolution with time of mean concentration, the continuous sinuous line represents the concentration without noise. The exact measurement of the dispersion around the mean is given by the standard deviation in Fig. 5, which is a plotter with the same variance parameter $q = 0.05$ at $x = 2.5$ (m), $x = 5$ (m) and $x = 5$ (m) in space. The mean concentration coincides with the deterministic solution, whereas the sample concentration oscillates above and below the mean concentration and the departure from the mean increases as time increases. The effect of stochasticity becomes greater with the distance from original increasing. Fig. 6 presents the situation when we increase the variance parameter to $q = 0.5$. We can see that the effect on the concentration becomes more obvious as q gets larger. The results indicate a Brownian type of behaviour, as we have expected.

A model like this presented in this section may partially explain the stochastic nature of the concentration in an aquifer. The information collected may help in the identification and parameter estimation of the stochastic process involved, and the model could be used to forecast the statistical properties of the concentration.

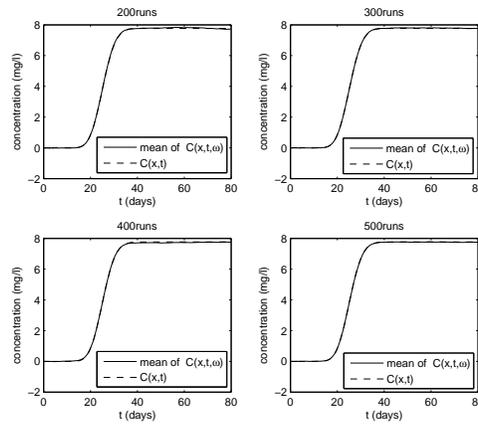


FIGURE 3. Stochastic concentration in space at $x = 5$ (m) from 200 runs to 500 runs, with $q = 0.05$.

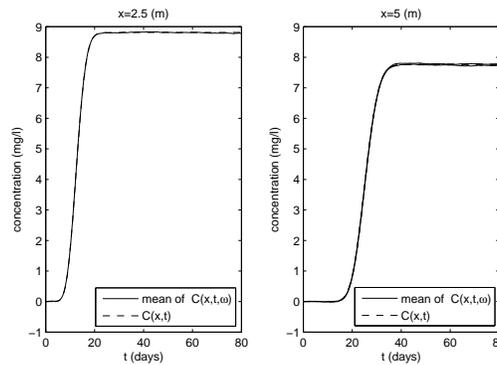


FIGURE 4. Stochastic concentration in space $x = 2.5$ (m) and $x = 5$ (m) from the origin in Case 1, with $q = 0.05$.

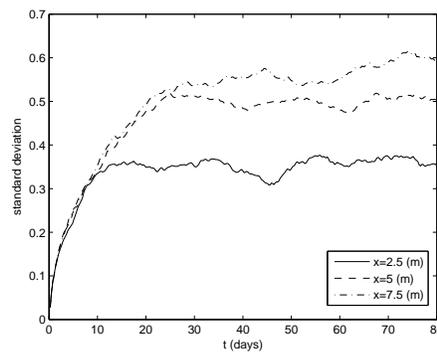


FIGURE 5. Standard deviation in space $x = 2.5$ (m), $x = 5$ (m) and $x = 7.5$ (m) from the origin in Case 1, with $q = 0.05$.

3.2. Case 2: A distributed source problem. Space stochasticity. Another interesting case arises when the function g in Eq. (1.2) is a stochastic process in space and smooth in time. This occurs when a source randomly distributes in time and

result which indicates a direct increase in the statistical dispersion of the concentration around the mean with time increasing. This implies that the time component is as important as the spatial component. Meanwhile they show a Brownian type of behaviour, as we have expected.

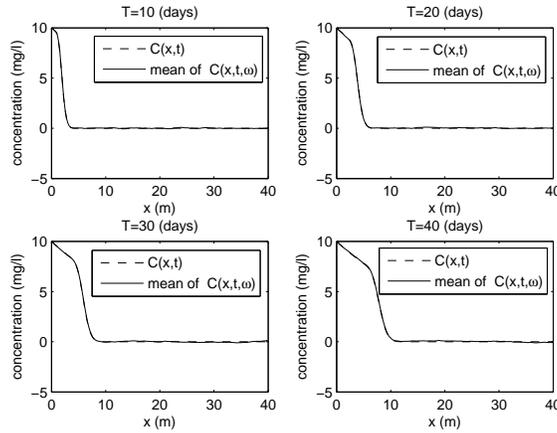


FIGURE 7. Stochastic concentration variation as time changes from 10 (days) to 40 (days) in Case 2, where $q = 0.01$.

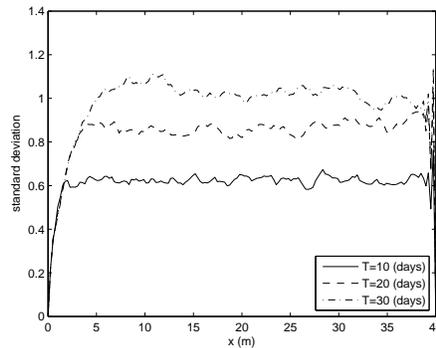


FIGURE 8. Standard deviation variation as time changes from 10 (days) to 30 (days) in Case 2, where $q = 0.01$.

3.3. Case 3: Stochasticity in the boundary conditions. We consider another important case where the boundary condition is a stochastic function in time. It appears in situation where there is a high degree of uncertainty with the history deposition of solid or liquid wastes in the groundwater system.

Let us consider the case of (1.1) when the function $k(t)$ is described by a white Gaussian process in time $\omega(t)$ with the properties described by (3.2):

$$(3.4a) \quad \frac{\partial C}{\partial t} - D \frac{\partial^2 C}{\partial x^2} + v \frac{\partial C}{\partial x} + \lambda C = 0,$$

$$(3.4b) \quad C(0, t) = w(t, \omega), \quad C(\infty, t) = 0, \quad C(x, 0) = 0.$$

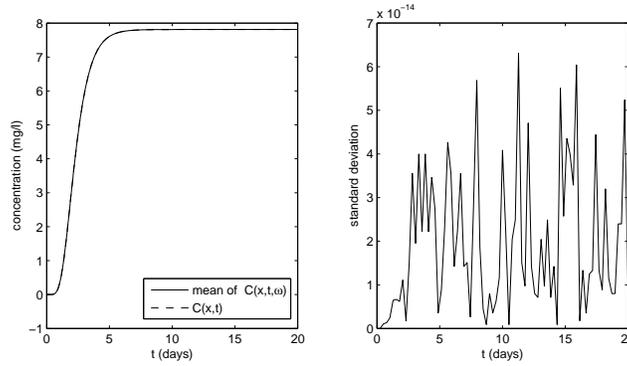


FIGURE 9. Stochastic concentration (left) and the standard deviation (right) of Case 3 at $x = 0.5$ (m) with $q = 0.1$.

This problem could be solved in space interval $[0, 10]$ and $T = 20$ (days). We take $N = 80$, $\Delta t = h^2$ as before. In our numerical simulations we add Gaussian noise $\omega(t)$ to produce the stochastic boundary condition $C(0, t) = C_0 + \omega(t)$. The other parameter values are the same as in Case 1 except the variance parameter q .

Fig. 9 and Fig. 10 show the stochastic evolution of the concentration with respect to time at $x = 0.5$ (m) and $x = 4.0$ (m) respectively with $q = 0.1$. Standard deviations are also given which have magnitudes of 10^{-14} and 10^{-15} respectively. That means time stochasticity at the boundary has little effect on the concentration. When we increase the variance parameter value to $q = 1$ in Fig. 11, the standard deviation has no obvious variation.

The results indicate that the effect of time stochasticity at the boundary decreases as the distance from the boundary increases. This of course depends on the type and variance of the disturbing process, but in general the concentration variance approaches to zero beyond several meters of distance from the boundary and the process is then governed by the mean source concentration. This indicates that the effect of stochasticity at the boundaries is relatively less important than the effect of distributed-source stochasticity on the overall stochasticity of the concentration distribution.

4. CONCLUSIONS

In this paper, we have numerically studied the advective-dispersive equation in the presence of stochastic force. In order to do so we design second-order finite volume element scheme for the considered problem. Numerical results demonstrate that the scheme can be used to solve advective-dispersive equation. In addition, the stochastic force would affect the distribution of contaminant concentration. Particularly, time stochasticity as a source term or spatial stochasticity as a source term have a stronger effect than time stochasticity in the boundary conditions.

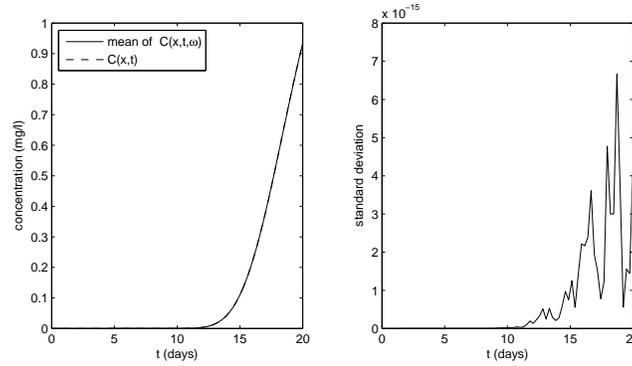


FIGURE 10. Stochastic concentration (left) and the standard deviation (right) of Case 3 at $x = 4.0$ (m) with $q = 0.1$.

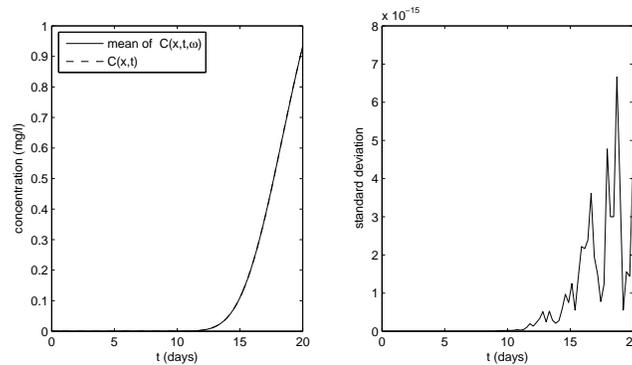


FIGURE 11. Stochastic concentration (left) and the standard deviation (right) of Case 3 at $x = 4.0$ (m) with $q = 1$.

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