MODELING OF SOLUTE TRANSPORT IN A HETEROGENEOUS POROUS MEDIUM WITH A RANDOM SOURCE USING STOCHASTIC FINITE ELEMENT METHOD

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Abstract

The randomness in the source condition other than the heterogeneity in the system parameters, can also be a major source of uncertainty in the concentration field. Hence, a more general form of the problem formulation is to consider both random source condition and system parameters. Under this condition, the response function becomes a random function and depends on the random system parameters. In the present study an attempt is made to include the system uncertainty and to assess the relative effects of system uncertainty and source uncertainty on the probabilistic behavior of concentration. Here the source is modeled as a random discrete process. The probabilistic behavior of the random response function is obtained by using a perturbation based stochastic finite element method. The proposed method is applied for analyzing the one dimensional solute transport problem considering hydraulic conductivity as a random field.

1. INTRODUCTION

Probabilistic studies of solute transport in porous media are mainly focused on predicting the concentration uncertainty due to the heterogeneity of the governing flow and transport parameters [Kapoor and Gelhar, 1994; Huang and Hu, 2000; Hassan 2001]. The input/source conditions can also be spatially and/or temporally varying random processes in a natural hydrologic system. Li and Graham [1999] considered the boundary condition due to recharge as a spatial/temporal random process. Recently, Wang and Zheng (2005) analyzed the contaminant transport under random sources in a deterministic groundwater system. In their model, the random source was considered either as a continuous source with random fluctuations in time or as a discrete instantaneous source.

During the solution of SPDE's when analytical methods are not applicable due to the complicated initial and source conditions, non-uniform flow fields and non-stationary parameters, numerical methods are often used. The popular and simple Monte Carlo Simulation Method (MCSM) is computationally exhaustive when a few thousands of realizations are required especially for higher degree of medium heterogeneities along with higher space-time grid resolution. To avoid this difficulty, alternate methods such as perturbation based stochastic finite element method (SFEM) [Chaudhuri and Sekhar, 2005] can be used. However, no problems are yet dealt combining random spatial parameter distributions with random sources using SFEM.

In the present study, a methodology using (SFEM) is proposed for solving flow and transport in a heterogeneous porous medium when both source conditions and system parameters are random. The source condition here is assumed as a Poisson process similar to the study of Wang and Zheng [2005], while hydraulic conductivity is treated as random fields. The probabilistic solution of concentration (i.e. mean and variance of concentration) for a unit pulse in such a stochastic system is obtained using SFEM, which is further used as a response function treating the source as a random process.

2. PROBABILISTIC ANALYSIS FOR HETEROGENEOUS SYSTEM

The governing equation for the transport of a linearly sorbing and decaying solute in a 1-D porous medium is given by,

$$\Big(n + \rho_b k_d\Big)\frac{\partial c(x,t)}{\partial t} + \frac{\partial}{\partial x}\Bigg(nv(x)c(x,t) - nD(x)\frac{\partial c(x,t)}{\partial x}\Bigg) = 0 \tag{1}$$

where $c(x,t)$ is the concentration at location x and time t. Here n and k_d are respectively spatially varying porosity and sorption. In Eq. (1), $v(x)$ is the pore water velocity vector which is defined as $v(x) = q(x)/n$. The seepage flux vector $q(x)$ is obtained using the hydraulic conductivity ($K(x)$) and hydraulic head ($h(x)$) based on the Darcy equation $q(x) = -K(x)\dfrac{\partial h(x)}{\partial x}$. Here $D(x)$ is the hydrodynamic dispersion coefficient, which is combined with molecular diffusion coefficient (D_m). The expression for it is given as, $D(x) = \alpha v(x) + D_m$. Here α is the local dispersivity. The flow is assumed to be at steady state. Using finite element method for spatial discretization and finite difference method (Crank-Nicholson formulation) for temporal discretization the global equation for transport with specified boundary conditions, is obtained as

$$[D_1]\{c^{t+1}\} = [D_2]\{c^t\} + \theta\{c_b^{t+1}\} + (1-\theta)\{c_b^t\}, \tag{2}$$

where the matrices $[D_1]$ and $[D_2]$ are function of system parameters. The global equation for the flow for a given head and flux boundary conditions is obtained as,

$$[K]\{h\} = \{h_0\}. \tag{3}$$

Here $[K]$ is the global hydraulic conductivity matrix in the flow equation. The velocity is obtained for a specified hydraulic head gradient.

In the perturbation based stochastic finite element method the concentration is expanded in a Taylor series about the value at mean of the random parameters (r'_p, $p = 1, 2, \cdots, N_r$) and can be expanded as follows:

$$\{c^{t+1}\} = \{c^{t+1}\}^{(0)} + \sum_{p=1}^{N_r}\{c^{t+1}\}^{(I)}_{r_p} r'_p + \frac{1}{2}\sum_{p=1}^{N_r}\sum_{q=1}^{N_r}\{c^{t+1}\}^{(II)}_{r_p r_q} r'_p r'_q \cdots . \tag{4}$$

Here $\Theta^{(I)}_{r_p} = \dfrac{\partial \Theta}{\partial r_p}$ and $\Theta^{(II)}_{r_p r_q} = \dfrac{\partial^2 \Theta}{\partial r_p \partial r_q}$. The derivatives of concentration for various orders can be expressed as,

$$\{c^{t+1}\}^0 = [\overline{D}_1]^{-1}\Big([\overline{D}_2]\{c^t\}^0 + \theta\{\overline{c}_b^{t+1}\} + (1-\theta)\{\overline{c}_b^t\}\Big), \tag{5}$$

$$\{c^{t+1}\}^I_{r_p} = [\overline{D}_1]^{-1}\Big(- [D_1]^I_{r_p}\{c^{t+1}\}^0 + [D_2]^I_{r_p}\{c^t\}^0 + [\overline{D}_2]\{c^t\}^I_{r_p}\Big), \tag{6}$$

$$\{c^{t+1}\}^{II}_{r_p r_q} = [\overline{D}_1]^{-1}\Big(- [D_1]^I_{r_p}\{c^{t+1}\}^I_{r_q} - [D_1]^I_{r_q}\{c^{t+1}\}^I_{r_p} + [D_2]^I_{r_p}\{c^t\}^I_{r_q} + [D_2]^I_{r_q}\{c^t\}^I_{r_p} + [\overline{D}_2]\{c^t\}^{II}_{r_p r_q}\Big). \tag{7}$$

The covariance matrix of the random parameters (which are piece-wise linear inside an element), are derived from the given variances and spatial correlation functions for the random fields. The equations and the procedure for obtaining stochastic quantities of velocity and dispersion coefficient are provided in detail in [Chaudhuri and Sekhar, 2006]. The correlation coefficient between the log hydraulic conductivity at any two points is given by, $\rho(x) = \exp\left(- \left(\frac{x}{\lambda}\right)^2\right)$, where λ is the correlation length.

3. RANDOM SOURCE CONDITION

The source is modeled as a sequence of instantaneous mass injection with random amount. The time interval of mass injection may be uniform or random. The total amount of cumulative mass in the system is the sum of random number of incidents: $\sum_{k=1}^{M(T)} c_{A_k}$, where $M(T)$ is the number of mass injections that occurred during the interval $[0, T]$. Here c_{A_k} is the amount of random mass injected at time τ_k. In finite element model, the concentration at i^{th} node ($c_i(t)$) due to a random source is obtained as,

$$c_i(t) = \sum_{k=1}^{M(T)} c_{A_k} G_{c_i}(t, \tau_k). \tag{8}$$

In the above expression, $G_{c_i}(t, \tau_k)$ is a response function of the concentration due to a unit mass of solute injected at time $t = 0$. When the governing transport parameters are also random fields, the Eq. (8) can be further expressed as,

$$c_i(t) = \sum_{k=1}^{M(T)} c_{A_k}\Bigg(\big(G_{c_i}(t,\tau_k)\big)^{(0)} + \sum_{p=1}^{N_r} \big(G_{c_i}(t,\tau_k)\big)^{(I)}_{r_p} r'_p + \frac{1}{2}\sum_{p=1}^{N_r}\sum_{q=1}^{N_r} \big(G_{c_i}(t,\tau_k)\big)^{(II)}_{r_p r_q} r'_p r'_q \Bigg) . \tag{9}$$

The random transport parameters are usually uncorrelated with the source conditions i.e. c_{A_k} and r'_p are uncorrelated. Since the random pulse input of concentration at two different times are independent, one can note that $\overline{c_{A_k} c_{A_l}} = (\overline{c}_A)^2 + \sigma^2_{c_A}\delta_{kl}$. Taking the expectation of the Eq. (9) the mean concentration is obtained as,

$$\overline{c}_i(t) = E[c_i(t)] = E\left[\sum_{k=1}^{M(T)} c_{A_k} G_{c_i}(t,\tau_k)\right] = \overline{c}_A A, \tag{10}$$

$$\text{where } A = \sum_{k=1}^{M(T)} \Bigg(\big(G_{c_i}(t,\tau_k)\big)^{(0)} + \frac{1}{2}\sum_{p=1}^{N_r}\sum_{q=1}^{N_r} \big(G_{c_i}(t,\tau_k)\big)^{(II)}_{r_p r_q} \overline{r'_p r'_q} \Bigg) \tag{11}$$

To obtain the cross covariance of concentration the expression of the expectation of the product of concentration at two different times and nodes is written as,

$$\begin{aligned}\overline{c_i(t_1)c_j(t_2)} = E[c_i(t_1)c_j(t_2)] &= E\Bigg[\sum_{k=1}^{M(T)}\sum_{l=1}^{M(T)} c_{A_k}c_{A_l}G_{c_i}(t_1,\tau_k)G_{c_j}(t_2,\tau_l)\Bigg] \\ &= \sigma_{c_A}^2 A_1 + (\overline{c}_A)^2 A_2. \end{aligned} \tag{12}$$

Here the terms A_1 and A_2 are obtained as,

$$\begin{aligned} A_1 = \sum_{k=1}^{M(T)} \Bigg(\big(G_{c_i}(t_1,\tau_k)\big)^{(0)}\big(G_{c_j}(t_2,\tau_k)\big)^{(0)} + \sum_{p=1}^{N_r}\sum_{q=1}^{N_r} \Bigg(\big(G_{c_i}(t_1,\tau_k)\big)^{(I)}_{r_p}\big(G_{c_j}(t_2,\tau_k)\big)^{(I)}_{r_q} \\ + \frac{1}{2}\Big(\big(G_{c_i}(t_1,\tau_k)\big)^{(0)}\big(G_{c_j}(t_2,\tau_k)\big)^{(II)}_{r_pr_q} + \big(G_{c_i}(t_1,\tau_k)\big)^{(II)}_{r_pr_q}\big(G_{c_j}(t_2,\tau_k)\big)^{(0)}\Big)\Bigg)\overline{r'_pr'_q}\Bigg). \end{aligned} \tag{13}$$

$$\begin{aligned} A_2 = \Bigg(\sum_{k=1}^{M(T)} \big(G_{c_i}(t_1,\tau_k)\big)^{(0)}\Bigg)\Bigg(\sum_{k=1}^{M(T)} \big(G_{c_j}(t_2,\tau_k)\big)^{(0)}\Bigg) + \frac{1}{2}\Bigg(\sum_{k=1}^{M(T)} G_{c_i}(t_1,\tau_k)\big)^{(0)}\Bigg) \\ \times\Bigg(\sum_{k=1}^{M(T)}\Bigg(\sum_{p=1}^{N_r}\sum_{q=1}^{N_r}\big(G_{c_j}(t_2,\tau_k)\big)^{(II)}_{r_pr_q}\overline{r'_pr'_q}\Bigg)\Bigg) + \frac{1}{2}\Bigg(\sum_{k=1}^{M(T)}\Bigg(\sum_{p=1}^{N_r}\sum_{q=1}^{N_r}\big(G_{c_i}(t_1,\tau_k)\big)^{(II)}_{r_pr_q}\overline{r'_pr'_q}\Bigg)\Bigg) \\ \times\Bigg(\sum_{k=1}^{M(T)}\big(G_{c_j}(t_2,\tau_k)\big)^{(0)}\Bigg) + \sum_{k=1}^{M(T)}\sum_{l=1}^{M(T)}\Bigg(\sum_{p=1}^{N_r}\sum_{q=1}^{N_r}\big(G_{c_i}(t_1,\tau_k)\big)^{(I)}_{r_p}\big(G_{c_j}(t_2,\tau_l)\big)^{(I)}_{r_q}\overline{r'_pr'_q}\Bigg). \end{aligned} \tag{14}$$

After further simplification, the cross covariance is obtained as,

$$\begin{aligned} \overline{c'_i(t_1)c'_j(t_2)} &= \overline{c_i(t_1)c_j(t_2)} - \overline{c}_i(t_1)\overline{c}_j(t_2) = \sigma_{c_A}^2 A_1 + (\overline{c}_A)^2 A_2 - (\overline{c}_A A)^2 \\ &= \sigma_{c_A}^2 A_1 + \sum_{k=1}^{M(T)}\sum_{l=1}^{M(T)}\Bigg(\sum_{p=1}^{N_r}\sum_{q=1}^{N_r}\big(G_{c_i}(t_1,\tau_k)\big)^{(I)}_{r_p}\big(G_{c_j}(t_2,\tau_l)\big)^{(I)}_{r_q}\overline{r'_pr'_q}\Bigg). \end{aligned} \tag{15}$$

Here the expectation of the product of more than two random varibles and the term $r'_pr'_q - \overline{r'_pr'_q}$ have been ignored, which results in the first-order accurate covariance matrix of concentration. In case random time interval between injection of source events is considered, then the statistical moments are obtained using the probability density function of the random time interval [Lin, 1967]. The mean concentration can be derived as,

$$\begin{aligned} \overline{c}_i(t) = E[c_i(t)] &= E\Bigg[\sum_{k=1}^{M(T)} c_{A_k}G_{c_i}(t,\tau_k)\Bigg] = E\Bigg[E\Bigg[\sum_{k=1}^{m} c_{A_k}G_{c_i}(t,\tau_k)\Bigg]\Bigg| M(T)=m\Bigg] \\ &= \sum_{m=0}^{\infty} P_M(m,T)E\Bigg[\sum_{k=1}^{m} c_{A_k}G_{c_i}(t,\tau_k)\Bigg] = \overline{c}_A A, \end{aligned} \tag{16}$$

$$\text{where } A = \lambda_p\int_0^T \Bigg(\big(G_{c_i}(t,\tau)\big)^{(0)} + \frac{1}{2}\sum_{p=1}^{N_p}\sum_{q=1}^{N_q}\big(G_{c_i}(t,\tau)\big)^{(II)}_{r_pr_q}\overline{r'_pr'_q}\Bigg)d\tau. \tag{17}$$

where λ_p is the expected number of events of mass injection per unit of time. The expectation of the product of concentration can be written as,

$$\overline{c_i(t_1)c_j(t_2)} = E[c_i(t_1)c_j(t_2)] = E\left[\sum_{k=1}^{M(T)} c_{A_k} G_{c_i}(t_1,\tau_k) \sum_{l=1}^{M(T)} c_{A_l} G_{c_j}(t_2,\tau_l)\right]$$

$$= \sum_{m=0}^{\infty} P_M(m,T) \sum_{k=1}^{m}\sum_{l=1}^{m} E\Big[c_{A_k}c_{A_l}G_{c_i}(t_1,\tau_k)G_{c_j}(t_2,\tau_l)\Big] = \Big((\overline{c}_A)^2 + \sigma_{c_A}^2\Big)A_1 + (\overline{c}_A)^2 A_2 \quad (18)$$

where the terms A_1 for $k = l$ and A_2 for $k \neq l$ are as follows:

$$A_1 = \lambda_p \int_0^T \Bigg(\big(G_{c_i}(t_1,\tau)\big)^{(0)} \big(G_{c_j}(t_2,\tau)\big)^{(0)} + \sum_{p=1}^{N_r}\sum_{q=1}^{N_r} \Bigg(\big(G_{c_i}(t_1,\tau)\big)_{r_p}^{(I)} \big(G_{c_j}(t_2,\tau)\big)_{r_q}^{(I)}$$
$$+\frac{1}{2}\Big(\big(G_{c_i}(t_1,\tau)\big)^{(0)}\big(G_{c_j}(t_2,\tau)\big)_{r_pr_q}^{(II)} + \big(G_{c_i}(t_1,\tau)\big)_{r_pr_q}^{(II)}\big(G_{c_j}(t_2,\tau)\big)^{(0)}\Big)\Bigg)\overline{r_p'r_q'}\Bigg) d\tau, \quad (19)$$

$$A_2 = \lambda_p^2 \int_0^T \big(G_{c_i}(t_1,\tau)\big)^{(0)} d\tau \int_0^T \big(G_{c_j}(t_2,\tau)\big)^{(0)} d\tau + \frac{\lambda_p^2}{2}\int_0^T G_{c_i}(t_1,\tau)\big)^{(0)} d\tau$$
$$\times \int_0^T \sum_{p=1}^{N_r}\sum_{q=1}^{N_r} \Big(\big(G_{c_j}(t_2,\tau)\big)_{r_pr_q}^{(II)}\overline{r_p'r_q'}\Big) d\tau + \frac{\lambda_p^2}{2}\int_0^T \sum_{p=1}^{N_r}\sum_{q=1}^{N_r}\Big(\big(G_{c_i}(t_1,\tau)\big)_{r_pr_q}^{(II)}\overline{r_p'r_q'}\Big)d\tau \quad (20)$$
$$\times \int_0^T \big(G_{c_j}(t_2,\tau)\big)^{(0)} d\tau + \lambda_p^2 \int_0^T\int_0^T \sum_{p=1}^{N_r}\sum_{q=1}^{N_r}\Big(\big(G_{c_i}(t_1,\tau_1)\big)_{r_p}^{(I)}\big(G_{c_j}(t_2,\tau_2)\big)_{r_q}^{(I)}\overline{r_p'r_q'}\Big) d\tau_1 d\tau_2.$$

The cross-covariance of concentration is obtained as,

$$\overline{c_i'(t_1)c_j'(t_2)} = \overline{c_i(t_1)c_j(t_2)} - \overline{c}_i(t_1)\overline{c}_j(t_2) = \Big((\overline{c}_A)^2 + \sigma_{c_A}^2\Big)A_1 + (\overline{c}_A)^2 A_2 - (\overline{c}_A A)^2 \quad (21)$$
$$= \Big((\overline{c}_A)^2 + \sigma_{c_A}^2\Big)A_1 + \lambda_p^2 \int_0^T\int_0^T \sum_{p=1}^{N_r}\sum_{q=1}^{N_r} \big(G_{c_i}(t_1,\tau_1)\big)_{r_p}^{(I)}\big(G_{c_j}(t_2,\tau_2)\big)_{r_q}^{(I)}\overline{r_p'r_q'} d\tau_1 d\tau_2.$$

In the expressions of (10) and (16) for mean and (15) and (21) for the covariance, the additional terms are derived using SFEM based on the covariance of random parameters and derivatives of concentration with respect to discretized random parameters. These terms include the effect of uncertainty in the governing parameters on probabilistic structure of concentration. The terms in the expressions of statistical parameters of concentration due to uniform and random time interval are very similar. The summation in the case of uniform time intervals are replaced with integration.

In Monte Carlo Simulation method (MCSM), for each realization the response function $(G_{c_i}(t,0))$ due to unit solute mass injection is obtained using a generated random vector of the discretized hydraulic conductivity field. A sequence of random solute mass and associated injection times are generated based on the specified statistical parameters of the source, to compute the concentration using Eq. (8). The ensemble mean and standard deviation of concentration are estimated from 10000 realizations.

4. RESULTS AND DISCUSSION

In a 1-D column the solute of unit concentration is assumed to be injected instantaneously and the transport of solute is considered due to advection and dispersion. The length of the column is $l = 1.0$ m. The solute is injected at $x = 0.1$ m and the concentration is measured at $x = 0.2$ m. The velocity for the deterministic system (homogeneous hydraulic conductivity field), is taken as, $v_d = 1.0$ m/day. The values of the governing parameters are chosen as, $n = 0.4$, $\rho_b k_d = 0.2$, $\alpha = 0.0025$ m and $D_m = 0.0025$ m^2/day. The correlation length is taken as $\lambda = 0.01$ m. The study has been performed for a range of coefficient of variation (COV) of hydraulic conductivity. Figure (1a) shows that the solute movement is slow for heterogeneous case since the effective velocity is less for the modeled random hydraulic conductivity field. The break through for the mean concentration obtained by SFEM and MCSM are matching well. The plot of standard deviation of concentration is with time (Fig. 1b) shows two peaks associated with rapid changes in mean concentration. This is expected since σ_{G_c} is computed from the derivative of $\bar{c}$. Based on the time interval and the amount of solute mass injected, the source condition

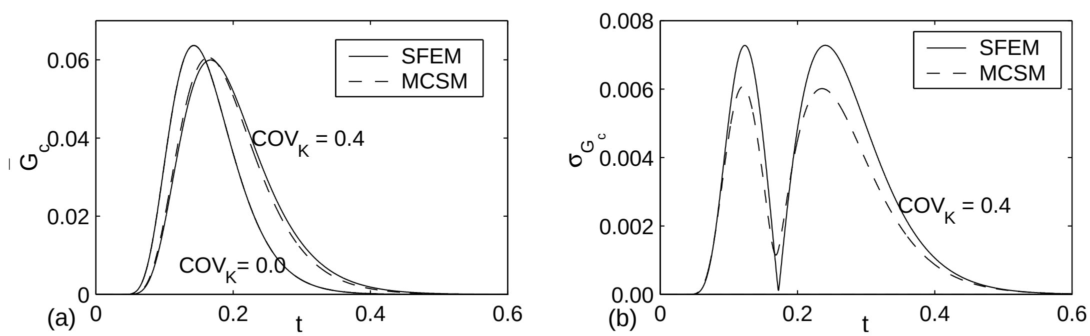

FIGURE 1. Comparison of mean and standard deviation of concentration obtained using SFEM and MCSM for unit mass injected.

is categorized into four cases as follows:

Case A - uniform time interval with fixed mass (COV$_{c_A} = 0.0$),
Case B - uniform time interval with random mass (COV$_{c_A} = 0.4$),
Case C - Random time interval (Poisson process) with fixed mass (COV$_{c_A} = 0.0$),
Case D - Random time interval (Poisson process) with random mass (COV$_{c_A} = 0.4$).
The expected number of mass injection per unit time is taken same for all the cases, $\lambda_p = 200$/day. The expressions in (Eqs. 10 and 16) show that the mean concentration is independent on the randomness in the amount of solute mass injected. It is shown in Figs. (2a) and (2b) that the mean concentration is same for both uniform and random time interval cases. If the time intervals between source injections are assumed to be large, then the mean break through of concentration shows oscillations. Since the theoretical analysis for deterministic system with random source condition is exact, the results match with Monte Carlo Simulation. As the area under the mean concentration break through (Fig. 1a) is higher, the steady state mean concentration happens to be higher

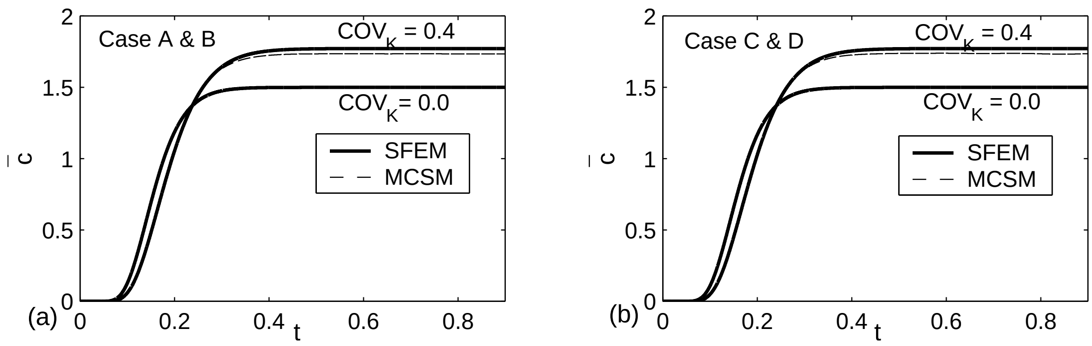

FIGURE 2. Comparison of mean of concentration obtained using SFEM and MCSM for various types of source conditions.

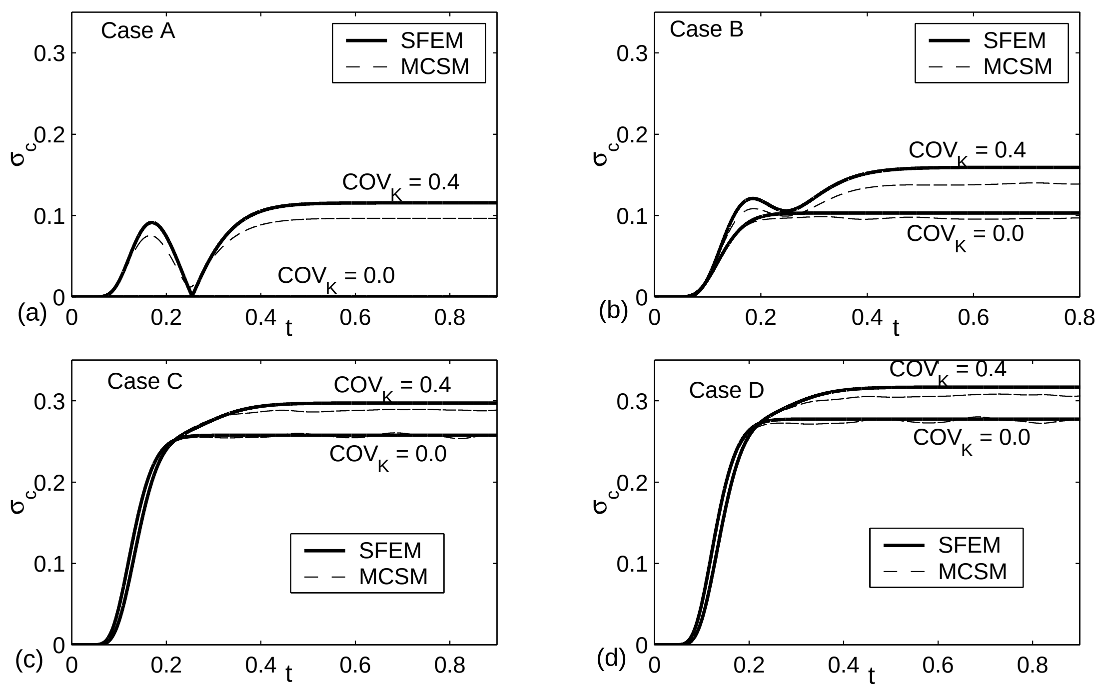

FIGURE 3. Comparison of standard deviation of concentration obtained using SFEM and MCSM for various types of source conditions.

for the heterogeneous system. The standard deviation of concentration for the deterministic source (Fig. 3a) shows a dip similar to single pulse input due to random hydraulic conductivity field (Fig. 1b). It increases monotonically with time as shown in Fig. (3b) when random amount of solute in injected at uniform time interval to a homogeneous column. The error with standard deviation is found to be more for random conductivity field. Figures (3c) and (3d) show that the standard deviation becomes significantly higher when the source is modeled as a Poisson process i.e. time interval follows an exponential distribution. Since the randomness in source injection dominates, the non-monotonic behavior due to random conductivity, is masked. Figure (4) shows that the concentration variance increases with COV of hydraulic conductivity. The increase of variance due to randomness in solute mass injected, is contributed by the term $(\sigma^2_{c_A} A_1)$ in the expressions of covariance (Eqs. 15 and 21). Comparing Eq. (15 and 21), it is interestingly observed that an additional term $((\overline{c}_A)^2 A_1)$ has appeared in Eq. (21) due to the Poisson process. The impact of this term is quite high as seen in Fig. (4). The similar effect due to various type of source conditions are observed as shown in Fig. (4) for the simulations with MCSM for $\mathrm{COV}_K = 0.4$.

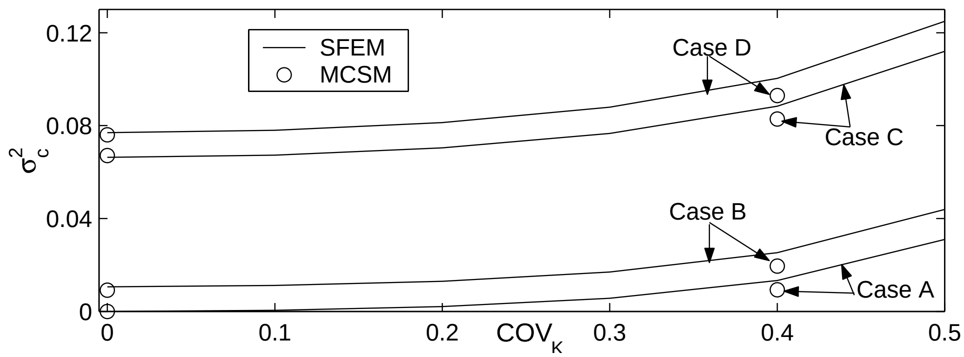

FIGURE 4. Relation between variance of concentration and COV of hydraulic conductivity for Cases A-D.

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