Stochastic finite element modeling of water flow and solute transport in unsaturated soils - a case-study

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Abstract

Hydrological processes are greatly influenced by the characteristics of the domain through which the process occurs. It is generally accepted that earth materials have extreme variations from point to point in space. Consequently this heterogeneity results in high variation in hydraulic properties of soil. In order to develop a predictive model for transport processes in soil, the effects of this variability must be considered. This paper presents the development a two-dimensional stochastic finite element model for simulation of water flow and solute transport in unsaturated soils. The model was validated with the data obtained from a field-scale irrigation furrow experiment. In this model, the perturbation-spectral based stochastic partial differential governing equation, obtained from classical Richard’s equation, is solved using a finite element method in the space domain and a finite difference scheme in the time domain. Effective hydrological parameters embedded in the mathematical model depend on time derivatives of capillary tension head. This makes possible consideration of the hysteresis due to large-scale variability of soil hydrological properties. A numerical scheme has been incorporated in the model to simulate infiltration and evaporation events and rapid changes in the boundary conditions (on the ground surface) from one type event to another one which commonly occurs in irrigation furrows. The results obtained from the model show better agreement with experimental measurements in comparison with deterministic HYDRUS-2D model. The possible reasons for this could be the consideration of the influence of the variability of the properties of soil and effects of parameter hysteresis on water flow and solute transport.

Keywords: stochastic finite element, heterogeneous soil, solute transport, unsaturated soil

1 Introduction

In recent years, interest in understanding the mechanisms and prediction of contaminant transport through soils has dramatically increased because of growing evidence and public concern that the quality of the subsurface environment is being adversely affected by industrial, municipal and agricultural activities. The movement of chemicals through the soil to the groundwater represents a degradation of these resources. So management of contaminated lands for control of groundwater quality will be a crucial requirement for sustainability. Contaminated land management and selection of appropriate and efficient remedial technologies are strongly dependent on the accuracy of predictive models in simulation of flow and solute transport in the soil. Recent studies have shown that current models and methods do not adequately describe the leaching of nutrients through soil, often underestimating the risk of groundwater contamination by surface-applied chemicals, and
overestimating the concentration of resident solutes (Stagnitti, et al., 2001). One of the most challenging problems in modeling of solute transport in soils is how to effectively characterize and quantify the uncertainties and the potential fluctuations in hydraulic parameters of the soil caused by natural heterogeneity of soil. Despite the many evidence from field-scale observations and experimental studies that show the significant effects of soil heterogeneity on contaminant transport (Al-Tabbaa, et al., 2000a; Smith, et al., 1996) these effects have been not included in the majority of the existing numerical models.

So the focus of this paper is development of a computationally efficient code using stochastic numerical method which is applicable to real world problems.

2 Stochastic finite element model

It is assumed that the local hydraulic properties which are randomly variable in space are realizations of three-dimensional, spatially correlated random fields. These random parameters are defined by combination of a mean value and possible perturbations around the mean. In a spectral based SFEM, for each element, the random parameters are decomposed as, 

$$ln k_i = F + f, \quad q = \bar{q} + q', \quad C = \bar{C} + C',$$

where $F$, $\bar{q}$ and $\bar{C}$ represent the mean values of saturated hydraulic conductivity, groundwater velocity and solute concentration, respectively and $f$, $q'$ and $C'$ represent the perturbations of saturated hydraulic conductivity, groundwater velocity and solute concentration. For a statistically homogeneous random field, the mean of the properties for each element remain the same. Hence, the matrices $[A]$ and $[D]$ are also decomposed into mean ($[\bar{A}]$ and $[\bar{D}]$) and zero mean fluctuating ($[A']$ and $[D']$) components including the zero mean random component of random variables, $r'_g$. Here $r'_g$, $(g=1,2,\ldots, N_r)$ are the velocity component, saturated hydraulic conductivity of each element. $N_r$ is total number of random variables. Expanding $[A]$ and $[D]$ using Taylor series and noting that 2nd and higher-order derivatives are negligible,

$$[D] = \bar{D} + D' = \bar{D} + \sum_{g=1}^{N_r} \frac{\partial [D]}{\partial r'_g} r'_g$$  \hspace{1cm} (2)

Therefore, the finite element equation is written as

$$[A]\left\{\begin{array}{c}
\frac{\partial \{\bar{C}\}}{\partial t} \\
\frac{\partial \{C\}'}{\partial t}
\end{array}\right\} + \left[\bar{D}\right] \left\{\begin{array}{c}
\{\bar{C}\} \\
\{C\}'
\end{array}\right\} + \left(\sum_{g=1}^{N_r} \frac{\partial [D]}{\partial r'_g} r'_g \right) \left\{\begin{array}{c}
\{\bar{C}\} \\
\{C\}'
\end{array}\right\} = \{C_0\}$$  \hspace{1cm} (3)

Averaging the equation (3) over the ensemble of possible realizations of the stochastic processes $r'_g$ yields the mean equation for solute transport. Therefore, the mean equation for solute transport is obtained through taking the expected value of this equation with respect to $r'_g$ as

$$[A]\left\{\begin{array}{c}
\frac{\partial \{\bar{C}\}}{\partial t} \\
\frac{\partial \{C\}'}{\partial t}
\end{array}\right\} + \left[\bar{D}\right] \left\{\begin{array}{c}
\{\bar{C}\} \\
\{C\}'
\end{array}\right\} + E \left(\sum_{g=1}^{N_r} \frac{\partial [D]}{\partial r'_g} r'_g \{C\}'\right) = \{C_0\}$$  \hspace{1cm} (4)

and the equation for the perturbed component of concentration is obtained by subtracting equation (4) from equation (5) as (Ghanem and Spanos, 2003)
\[
\left[ A \right] \frac{\partial \hat{\mathbf{C}}}{\partial t} + \left( \left[ D \right] \hat{\mathbf{C}} + \sum_{g=1}^{N_{r}} \frac{\partial \left[ D \right]}{\partial r_{g}} r_{g} \hat{\mathbf{C}} \right) = 0
\]  

(5)

where \( E \left( \sum_{g=1}^{N_{r}} \frac{\partial \left[ D \right]}{\partial r_{g}} r_{g} \hat{\mathbf{C}} \right) \) represents the dynamic transport matrix produced under the effects of spatial variability of hydraulic parameters. Spectral theory can be used to evaluate the above expected value and the solute concentration variance. As the fluctuations of soil hydraulic properties are assumed to be realizations of stationary random fields, they can be expressed in the wave number domain as \( r_{g} = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{i k \cdot x} dZ_{r g} \), where \( k \) is the wave number vector, \( i \) is imaginary unit \((i^2 = -1)\) and \( dZ_{r g} \) is Fourier-Stieltjes spectral amplitude of \( r_{g} \) (Mantoglou and Gelhar, 1987). So the random fluctuations are expressed in the wave number domain. Then following properties of the amplitudes of cross-correlated stationary random variables (Lumley and Panofsky, 1964) are used to present the spectral density function of random input parameters as function of spectral density function of \( k_{r} \).

\[
E \left[ dZ_{r g} (k_1) dZ_{r g}^{*} (k_2) \right] = S_{r g} (k) dk \quad \text{if } k_1 = k_2 = k
\]

\[
E \left[ dZ_{r g} (k_1) dZ_{r g}^{*} (k_2) \right] = 0 \quad \text{otherwise}
\]

(6)

Therefore, the arrays of the dynamic transport matrix of fluctuations based on saturated hydraulic conductivity with a log-normal distribution assumed \( K_{s} \) and an anisotropic exponential covariance function are given by Gellar and Axness, (1983) as

\[
D'_{ij} = \int_{k} \frac{k_i^2 J_{m} J_{n} \left( \delta_{im} - k_i k_n / k^2 \right) \left( \delta_{jn} - k_i k_n / k^2 \right) \left( S_{ij} (k) \right) dk}{q^2 \left[ i k_i + \alpha_i k_i^2 + \alpha_r \left( k_2^2 + k_3^2 \right) \right]}
\]

(7)

where \( S_{ij} (k) = \sigma_{ij}^2 \lambda_{i} \lambda_{j} \lambda_{3} / \left[ \pi^2 \left( 1 + k_1^2 \lambda_{1}^2 + k_2^2 \lambda_{2}^2 + k_3^2 \lambda_{3}^2 \right) \right] \), \( \lambda \) is correlation length and \( \sigma_{ij}^2 \) is the variance of \( k_{s}, J \) is the pore water pressure gradient and \( \delta \) is the Kronecker delta.

The expression for variance of solute concentration is obtained as (Vomvoris and Gelhar, 1990):

\[
\sigma_c^2 = \int_{-\infty}^{\infty} G_{s} G_{e} e^{2F} J_{m} J_{n} \left( \delta_{jm} - k_j k_m / k^2 \right) \left( \delta_{jn} - k_j k_n / k^2 \right) S_{ff} \frac{q^2 \left[ k_i^2 + \left( \alpha_i k_i^2 + \alpha_r \left( k_2^2 + k_3^2 \right) \right) \right]}{q^2 \left[ k_i^2 \left( i k_i + \alpha_i k_i^2 + \alpha_r \left( k_2^2 + k_3^2 \right) \right) \right]}
\]

(8)

where, \( G_{s} = -\frac{\partial \hat{C}}{\partial x} \) is the mean concentration gradient. Summation over \( m \) and \( n \) is implied. Applying a finite difference scheme (Stasa, 1985) to equation (4) yields
\[
[A]\left\{\left(\begin{array}{c}
\hat{C} \\
\hat{\theta}
\end{array}\right)^{t+\Delta t}\right\} + \left(\begin{array}{c}
\hat{C} \\
\hat{\theta}
\end{array}\right)^{t} - \frac{\left(\begin{array}{c}
\hat{C} \\
\hat{\theta}
\end{array}\right)^{t}}{\Delta t}\right\} \\
+ [D]\left(\begin{array}{c}
\hat{C} \\
\hat{\theta}
\end{array}\right)^{t+\Delta t} + E\left(\sum_{g=1}^{N_{p}}[D]_{rg}r_{g}\left(\begin{array}{c}
\hat{C} \\
\hat{\theta}
\end{array}\right)^{t+\Delta t}\right) = \{C_0\}
\]

(9)

where \(\Delta t\) is the time step; \(t\) represents the time level.

3 Model validation and case study

The developed stochastic finite element model has already been verified against the results obtained from the Monte Carlo method for steady-state flow and transient contaminant transport (Nezhad and Javadi, 2009). Here, it is verified for the case of transient flow and contaminant transport by simulation of a field-scale solute transport problem (Abbasi, et al., 2003a; Abbasi, et al., 2003b). The case study involves a field experiment, conducted by Abbasi et al., (2003a) at the Maricopa Agricultural Center in Phoenix, AZ, in order to investigate the distribution of soil moisture and solute concentration in the soil profile below and adjacent to the agricultural irrigation furrows. The length of furrows is 115 m. Two sets of neutron probe access tubes were installed at \(x = 5\) and \(110\) m along the monitored furrow. Hereafter we refer to these locations as the inlet and outlet sites, respectively. Soil samples for gravimetric soil water content were collected 12 hours and five days after the irrigation at three different locations: at 5 and 110 m (the inlet and outlet sites, respectively). The samples were taken from one side of the monitored furrows at three locations (top, side, and bottom of the furrow; e.g. at locations 1, 2 and 3 in Fig. 1) in a cross-section perpendicular to the furrow axis. Water flow depths in the furrows were taken at the inlet and outlet sites every few minutes as soon as A free-drainage condition for water was applied to the lower boundary of the domain (Fig. 1). No-flux boundary conditions were applied to both sides of the flow domain. Bromide in the form of CaBr\(_2\) was injected at a constant rate of 6.3 g Br/l during the entire irrigation. A Cauchy boundary condition was used for the upper boundary for solute transport. The mean value for the scaling parameter (\(\alpha\)) is equal to 3.9 l/m with a variance equal to 0.8 l/m\(^2\). The vertical correlation scale was considered equal to 0.2 m.

Time- and space-dependent flow depths (surface ponding, \(h(x,t)\) in Fig. 1) were specified as the upper boundary condition in the furrow during irrigation. Time- and space-dependent flow depths (surface ponding, \(h(x,t)\) in Fig. 1) were specified as the upper boundary condition in the furrow during irrigation.

The variances of stochastic parameters and the vertical correlation length values assumed different values combination that produced the closest results to experimental results (Results were not presented here). Also the results of sensitivity analysis with regards to variance of stochastic parameters show that the increase of variances as an index of soil heterogeneity results in the higher rate of diffusion of solute. The measured and predicted values (using the SFE model developed in this study and HYDRUS2-D model (Simunek, et al., 1999) of Bromide concentration at the inlet and outlet sites of the experiment are presented in Fig. 2. The computations for this problem were performed on a Microsoft Windows® XP Vista TM, on an Intel® Pentium® Dual CPU E2200 @ 2.20GHz processor. It was found that the computation time taken for this problem was about 4 hours. The results are given by means of 1D curves to provide a better visual comparison between the measured and calculated distributions. The solid and dashed lines show simulation results obtained by HYDRUS-2D in combination with simultaneous and two-step optimization approaches, respectively (Abbasi, et al., 2004). The symbols \(\times\) show the results obtained using the stochastic finite element model. From comparison of the results, it is concluded that stochastic the finite element method...
Figure 1. Boundary conditions used for numerical modelling.

Table 1. Parameter values used for the numerical simulations

<table>
<thead>
<tr>
<th>Site</th>
<th>Site</th>
<th>$K_z$ (m/s)</th>
<th>$\sigma_f^2$</th>
<th>$\alpha_L$ (m)</th>
<th>$\alpha_T$ (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Simultaneous</td>
<td>Inlet</td>
<td>$1.39 \times 10^{-3}$</td>
<td>$2.22 \times 10^{-1}$</td>
<td>$4.4 \times 10^{-2}$</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Outlet</td>
<td>$1.59 \times 10^{-3}$</td>
<td>$9.1 \times 10^{-2}$</td>
<td>$1.0 \times 10^{-4}$</td>
<td></td>
</tr>
<tr>
<td>Two-step optimization</td>
<td>Inlet</td>
<td>$7.6 \times 10^{-4}$</td>
<td>$2.005 \times 10^{-3}$</td>
<td>$4.34 \times 10^{-2}$</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Outlet</td>
<td>$1.78 \times 10^{-3}$</td>
<td>$1.74 \times 10^{-2}$</td>
<td>$4.0 \times 10^{-4}$</td>
<td></td>
</tr>
<tr>
<td>SFE</td>
<td>Inlet</td>
<td>$1.5 \times 10^{-3}$</td>
<td>$0.6$</td>
<td>$2.0 \times 10^{-1}$</td>
<td>$2.0 \times 10^{-2}$</td>
</tr>
<tr>
<td></td>
<td>Outlet</td>
<td>$1.5 \times 10^{-3}$</td>
<td>$0.6$</td>
<td>$2.0 \times 10^{-1}$</td>
<td>$2.0 \times 10^{-2}$</td>
</tr>
</tbody>
</table>

Figure 2. Measured and predicted (using SFE and HYDRUS2-D models) Bromide concentration for the inlet and outlet sites (measured: •, simultaneous: solid lines, two-step: dashed lines, SFE: ×).
Produced better agreement with the observed concentrations, than HYDROUS-2D. HYDROUS-2D is a deterministic numerical code and the effects of spatial variability of soil hydraulic parameters are not considered in this model.

4 Conclusions

This paper presented a coupled transient SFE model for predicting the flow of water and contaminant transport in unsaturated soils. The model was validated by application to a real field scale case study with the aim of studying the effects heterogeneity of soil on contaminant concentration and transport. The SFE model performed well in predicting transport of contaminants through the soil. Comparison of the results of the SFE and DFE models with the experimental results shows that the SFE model is capable of predicting the solute transport with higher accuracy than DFE.

References


