

Uncertainty analysis of transient unsaturated flow in bounded domain

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[1] This paper analyzes the head variance during transient flows in unsaturated porous media. The analysis is based on a first-order Taylor series expansion of the discretized Richards' equation and stochastic conceptualization of hydrologic properties in space. Effects of boundary conditions and flow conditions (drying or wetting) were examined for different soil models. Results of the study indicate that a constant flux boundary condition affected the pressure head variance distribution close to the surface, originating a decrease of the values at early times during wetting scenarios. On the other hand, a constant head boundary condition strongly affected the variance profiles during both transient and steady flows, also far from the boundary. *INDEX TERMS:* 1869 Hydrology: Stochastic processes; 1875 Hydrology: Unsaturated zone; *KEYWORDS:* unsaturated zone; stochastic process

1. Introduction

[2] During the last 2 decades many stochastic theories have been developed to investigate the uncertainty in prediction of unsaturated flow due to spatial variation of the hydraulic characteristics of soils [e.g., Yeh *et al.*, 1985a, 1985b; Mantoglou and Gelhar, 1987a, 1987b; Yeh, 1989; Harter and Yeh, 1996; Yeh, 1998]. However, analysis of effects of heterogeneity on transient unsaturated flow is generally limited [e.g., Ferrante and Yeh, 1999; Li and Yeh, 1998; Zhang and Winter, 1998]. In this study, a numerical model is used to evaluate the variation of the pressure head variance in time and space in soils described by different soil models under wetting and drying processes under flux or head boundary conditions.

2. Numerical Model

[3] The one-dimensional (1-D), h -based Richards' equation is generally used to predict the flow in unsaturated soils:

$$\frac{\partial}{\partial z} \left[K(h) \frac{\partial(h-z)}{\partial z} \right] = C(h) \frac{\partial h}{\partial t}, \quad (1)$$

where z is the positive downward vertical coordinate, K is the hydraulic conductivity, h is the soil water pressure head, $C(h) = \partial\theta/\partial h$ is the specific moisture capacity, and θ is the moisture content; h is negative for unsaturated flow.

[4] Because (1) is a nonlinear, parabolic, partial differential equation, analytic solution is possible only for some special cases. Therefore numerical methods are typically used to integrate the Richards' equation. Using a fully implicit finite element scheme, (1) can be expressed in a matrix form [Bao, 1995]:

$$\mathbf{P}(\mathbf{h}_i, \mathbf{p})\mathbf{h}_i = \mathbf{Q}(\mathbf{h}_i, \mathbf{p})\mathbf{h}_{i-1} + \mathbf{f}(\mathbf{h}_i, \mathbf{p}, \mathbf{u}). \quad (2)$$

In (2), \mathbf{h}_i is the vector of head values at the time t_i at n nodes, where the subscript i denotes the time level; \mathbf{p} is the vector of the m parameters used to define the soil hydraulic properties; and \mathbf{u} is the

boundary condition vector. \mathbf{P} is the matrix associated with K and \mathbf{Q} terms evaluated at \mathbf{h}_i , while \mathbf{Q} is the matrix associated with the \mathbf{C} terms evaluated at \mathbf{h}_i . The vector \mathbf{f} is related to the boundary conditions and the gravity term.

[5] As shown by Ferrante and Yeh [1999], expanding (2) in Taylor series around the mean up to the first order and taking the expected value, the following approximate mean equation is obtained:

$$\mathbf{P}(\langle \mathbf{h}_i \rangle, \langle \mathbf{p} \rangle) \langle \mathbf{h}_i \rangle = \mathbf{Q}(\langle \mathbf{h}_i \rangle, \langle \mathbf{p} \rangle) \langle \mathbf{h}_{i-1} \rangle + \mathbf{f}(\langle \mathbf{h}_i \rangle, \langle \mathbf{p} \rangle, \langle \mathbf{u} \rangle), \quad (3)$$

where values within angle brackets denote the expected value of variables and parameters. Equation (3) is the mean equation of the first-order analysis, and it agrees with (1) if the mean values for the parameters and the variables are used.

[6] Subtracting (3) from the Taylor expansion of (2) up to the first order results in a perturbation equation. The perturbation equation can be used to evaluate the head covariance matrix \mathbf{R}_{hh} in terms of the parameter and boundary condition covariance matrices, \mathbf{R}_{pp} and \mathbf{R}_{uu} , respectively. Assuming that the soil parameters and the boundary conditions are uncorrelated, the head covariance equation can be written as [Ferrante and Yeh, 1999]:

$$\mathbf{R}_{hh} = \langle \mathbf{h}'_i \mathbf{h}'_i{}^T \rangle = \mathbf{B}_i \mathbf{R}_{pp} \mathbf{B}_i^T + \mathbf{C}_i \mathbf{R}_{uu} \mathbf{C}_i^T. \quad (4)$$

\mathbf{B}_i and \mathbf{C}_i matrices depend on matrices \mathbf{P} , \mathbf{Q} , and \mathbf{f} and on their derivatives with respect to \mathbf{h}_{i-1} and \mathbf{h}_i . Terms in the \mathbf{R}_{pp} covariance matrix depend on the parameters that are used to define the soil hydraulic properties and on their covariance and cross-covariance functions. The boundary condition covariance matrix, \mathbf{R}_{uu} , is a two-by-two matrix with the variance of the boundary condition on the diagonal and zero on the off-diagonal terms. Notice that (3) and (4) are based on the first-order approximation, implying the spatial variability of unsaturated hydraulic conductivity is small so that higher-order terms can be neglected.

3. Simulation Conditions

[7] The solution of (1) requires the specification of $K(h)$ and $\theta(h)$. Many models have been used in the past for this purpose. For

Table 1. Deterministic Parameter Values and Equation Numbers Corresponding to the Soil Models Used

	I	K_s , cm min ⁻¹	α_{is} cm ⁻¹	β_i	θ_s , cm ³ cm ⁻³	θ_r , cm ³ cm ⁻³	Equation	
							$K(h)$	$\theta(h)$
Gardner-Russo	GR	7.4203×10^{-5}	2.3861×10^{-2}		0.1946	0.0946	(5)	(6)
Gardner-exponential	GE	7.4203×10^{-5}	2.3861×10^{-2}		0.4196	0.0946	(5)	(7)
Gardner-linear	GL	7.4203×10^{-5}	2.3861×10^{-2}	3.2139×10^{-4}	0.4196		(5)	(8)
van Genuchten	vG	2.7825×10^{-2}	4.9529×10^{-2}	1.8109	0.4196	0.1342	(9)	(10)
Brooks and Corey	BC	2.7825×10^{-2}	7.9303×10^{-2}	0.6384	0.4717	0.1342	(11)	(12)

example, the *Gardner* [1958] soil model describes the constitutive relationship between K and h with an exponential function:

$$K(h) = K_s e^{\alpha_G h}. \quad (5)$$

K_s is the saturated hydraulic conductivity, and α_G is a parameter related to the soil pore distribution. *Russo* [1988] derived a parametric expression for the soil constitutive relationship, $\theta(h)$, consistent with *Mualem's* [1976] theory:

$$\theta(h) = \theta_r + (\theta_s - \theta_r) \left[e^{\alpha_{GR} h/2} (1 - \alpha_{GR} h/2) \right]^{2/(m+2)}, \quad (6)$$

where θ_s and θ_r are the saturated and residual water contents, respectively, and m is a parameter that accounts for the dependence of the tortuosity, usually set to be 0.5. *Mantoglou and Gelhar* [1987a, 1987b], in their stochastic analysis of transient flow in unsaturated soils, used a linear relationship between θ and h :

$$\theta = \theta_s + \beta_{GL} h. \quad (7)$$

This model leads to a constant value, β_{GL} , for the specific soil moisture capacity, $C(h)$. An exponential relationship for the moisture content, similar to that proposed by *Russo* [1988], was used by *Srivastava and Yeh* [1991]:

$$\theta(h) = \theta_r + (\theta_s - \theta_r) e^{\alpha_{GE} h}. \quad (8)$$

This model linearizes the Richards' equation such that closed-form analytical solutions become possible.

[8] The soil model proposed by *Brooks and Corey* [1964] is based on the empirical relationships:

$$\theta(h) = \begin{cases} (\theta_s - \theta_r) (-\alpha_{BC} h)^{-\beta_{BC}}, & |h| < 1/\alpha_{BC} \\ (\theta_s - \theta_r), & |h| \geq 1/\alpha_{BC} \end{cases} \quad (9)$$

$$K(h) = \begin{cases} K_s (-\alpha_{BC} h)^{-(2+3\beta_{BC})}, & |h| < 1/\alpha_{BC} \\ K_s, & |h| \geq 1/\alpha_{BC} \end{cases} \quad (10)$$

where α_{BC} is the inverse of the air-entry pressure head value. Another popular soil model is the one by *van Genuchten* [1980]:

$$\theta(h) = \left\{ 1 / [1 - (\alpha_{vG} |h|)]^{\beta_{vG}} \right\}^{1-(1/\beta_{vG})} \quad (11)$$

$$K(h) = K_s \frac{\left\{ 1 + (\alpha_{vG} |h|)^{n-1} [1 - (\alpha_{vG} |h|)^n]^{-1+(1/\beta_{vG})} \right\}^2}{[1 - (\alpha_{vG} |h|)^{\beta_{vG}}]^{m[1-(1/\beta_{vG})]}} \quad (12)$$

The Brooks and Corey (BC) and the van Genuchten (vG) soil models, (9) and (10) and (11) and (12) respectively, have more

parameters than those based on the Gardner equation. They generally fit the experimental data better over a wide range of h values. The Gardner-Russo (GR) model as well as the Gardner exponential (GE) and the Gardner linear (GL) models, because of their simplicity, are commonly used to derive analytical solutions for the deterministic and stochastic analysis of flow in unsaturated soils.

[9] The five different soil models are used in the following numerical analysis to investigate the evolution of head variation during drying and wetting processes under different boundary conditions in a vertical, one-dimensional, heterogeneous soil profile. At the soil surface a constant flux or a constant head boundary condition is used, and at the bottom boundary a water table is specified. The total length of the soil profile, 5000 cm, is divided into 250 elements with a length of 20 cm each. Soil parameter $f = \log(K_s/\langle K_s \rangle)$ is assumed to be second-order stationary Gaussian stochastic process. An exponential covariance function with an integral scale ($\lambda = 250$ cm) is used for f .

[10] Mean values for parameters of the five soil models are given in Table 1. The parameter values of the vG model are identical to those of the Bet Dagan soil [*Russo and Bouton*, 1992]; the parameter values of the remaining four models were derived from matching their shapes to that of the vG model.

[11] For the three soil models based on the Gardner $K(h)$ function, the matching is based on the minimization of the area enclosed between two curves, bounding the parameter values to

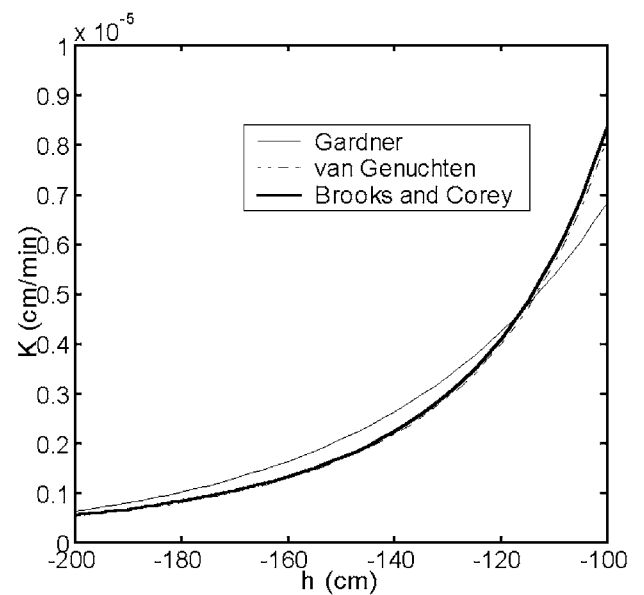


Figure 1. Hydraulic conductivity functions, $K(h)$, for the different soil models in the pressure head range considered in the simulations.

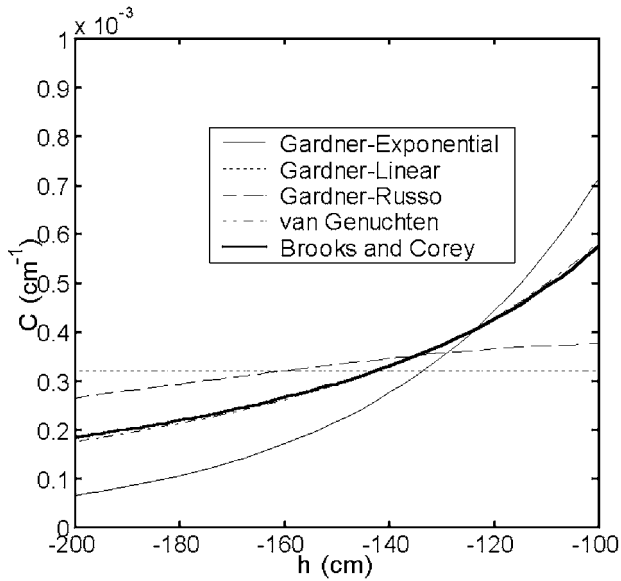


Figure 2. Specific moisture capacity functions, $C(h)$, for the different soil models in the pressure head range considered in the simulations.

have a physical meaning (i.e., positive values, $\theta_s > \theta_r$, etc.). The conversion method proposed by *Ma et al.* [1999] was used for the BC soil model. The $K(h)$ and $C(h)$ functions are shown in Figures 1 and 2, respectively, for the five different soil models.

[12] In order to compare front propagation in wetting and drying cases, two flux values are chosen for the constant flux boundary condition, $q_a = 7.469 \times 10^{-6}$ and $q_b = 5.792 \times 10^{-7}$ cm/min, respectively. A wetting front is originated by changing the flux at $t = 0$ from q_b to q_a , while the drying front is originated by changing it from q_a to q_b until a final steady state condition is obtained. For the prescribed head surface boundary conditions those head values corresponding to the steady state unit gradient distribution for q_a and q_b are chosen. In this manner a variation of the mean pressure head ranging approximately from -200 to -100 cm is obtained for all the cases considered. The initial conditions for these cases are the steady state pressure head profiles corresponding to the prescribed initial boundary flux or head conditions.

4. Results and Discussion

[13] Figure 3a depicts mean head profiles at several time intervals during a drying scenario, produced by a change of the flux boundary condition at the surface. In Figure 3a the normalized distance from the surface, $z^* = z/\lambda$ is used and times $t_0, t_1, t_2,$ and t_3 , refer to 0 min, 2.5×10^6 min, 7.5×10^6 min, and 22.5×10^6 min, respectively. Differences in front propagation velocity and diffusive front are evident in Figure 3a for the five soils, when the front position in time and the maximum pressure head gradient in space are compared. Initial and final steady state profiles coincide for the three soil models GE, GL, and GR, because they share the same Gardner constitutive function and the $C(h)$ function does not affect the steady state profile.

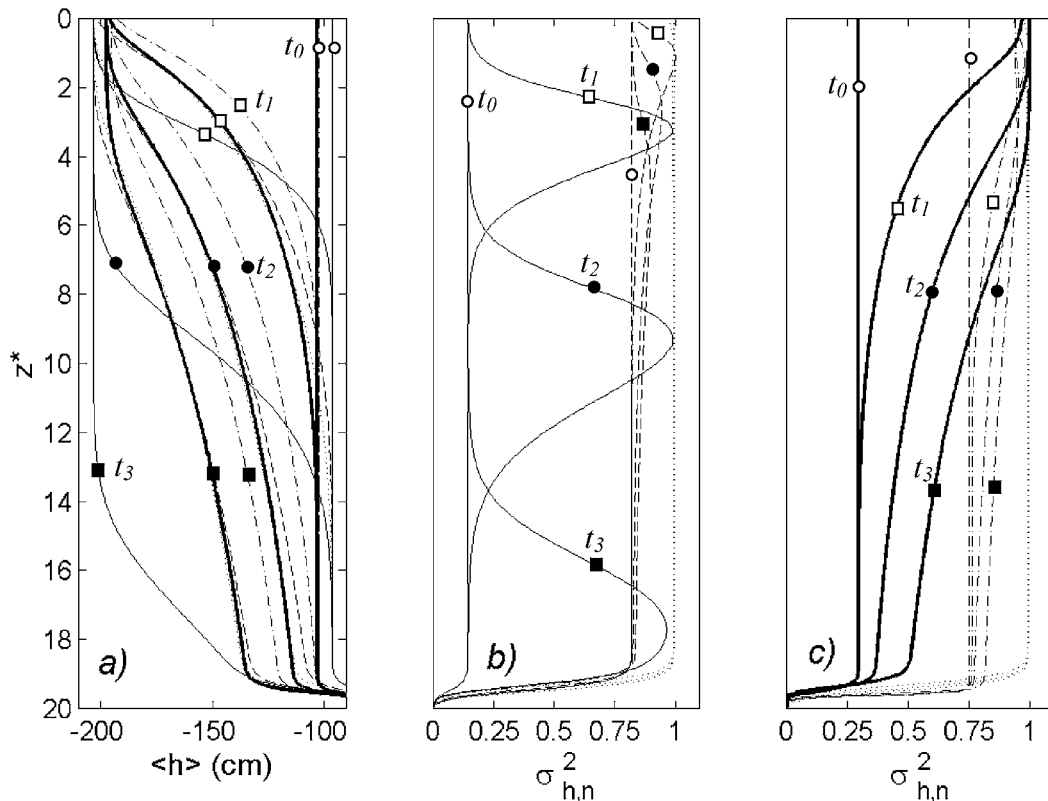


Figure 3. (a) Mean pressure head and (b and c) normalized pressure head variance profiles for the Gardner exponential (GE) (solid bold curves), Gardner linear (GL) (dotted curves), Gardner-Russo (GR) (dashed curves), van Genuchten (vG) (dashed-dotted curves), and Brooks and Corey (BC) (solid thin curves) soil models for a drying scenario and a constant flux top boundary condition.

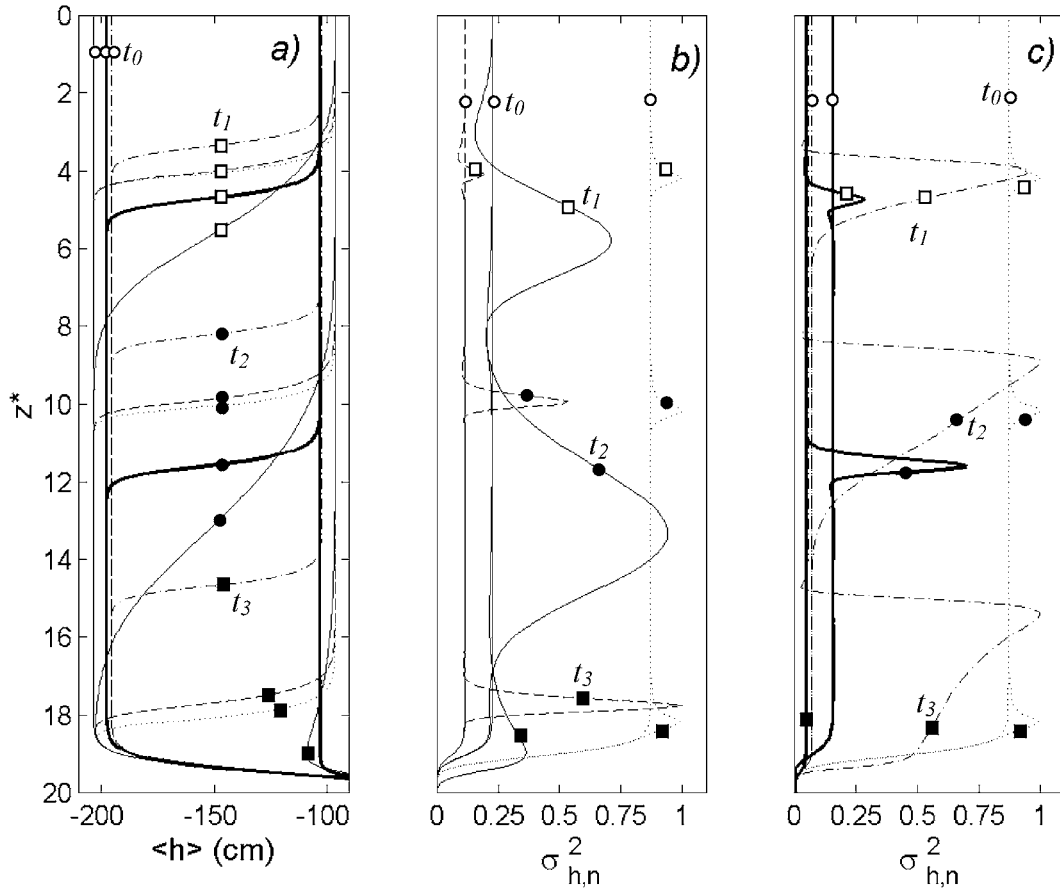


Figure 4. (a) Mean pressure head and (b and c) normalized pressure head variance profiles for GE (solid bold curves), GL (dotted curves), GR (dashed curves), vG (dashed-dotted curves), and BC (solid thin curves) soil models for a wetting scenario and a constant flux top boundary condition.

[14] Initial mean pressure head profiles for vG and BC soils are very similar to each other. Differences between these initial steady state profiles and those for the other soil models are attributed to differences in K values for different constitutive functions (see $K(-100)$ and $K(-200)$ values for Gardner, BC, and vG models in Figure 1). Although vG and BC constitutive functions are very similar, still differences in the front propagation velocity are evident comparing the mean pressure head profiles for the soil models at a given time.

[15] In Figure 3b, pressure head variances due to the uncertainty of f values are shown for the pressure head profiles in Figure 3a, for GE, GR, and GL models. For a better comparison the normalized variance of h , $\sigma_{h,n}^2 = \sigma_h^2 / (\sigma_f^2 \sigma_{h,\max}^2)$, is plotted, where $\sigma_{h,\max}^2$ is the maximum of σ_h^2 during front propagation in each soil. Since soil parameters and boundary conditions are uncorrelated and the numerical model is linear with respect to parameter variances, the normalization with respect to σ_f^2 makes the results independent of the σ_f^2 value used. The profile for $t = 0$ corresponds to the stochastic initial steady state condition, originated by the deterministic boundary conditions in the soil with stochastic hydraulic properties. The initial steady state pressure head variance value is in a good agreement with the analytical solution by Yeh [1989]. We find that initial and final steady state pressure head variance profiles are exactly the same for each of the three soil models GE, GL, and GR, independently of the mean pressure head value. This finding is consistent with that of Yeh [1989], for Gardner soil model under steady state conditions, when only f is

a stochastic variable. As for the mean pressure head profile, the σ_h^2 of the steady state profile for the three soils is exactly the same.

[16] Peaks of the pressure head variance under transient conditions are found at the locations of the maximum head gradient. Their values usually increase with time. The smaller diffusion front for GR and GL soil models, comparing to GE, yields a narrower pressure head variance “wave.”

[17] In Figure 3c profiles of normalized pressure head variance are shown for GL, vG, and BC soil models. The general behavior is similar to that described in Figure 3b, but for initial and final steady state pressure head variance profiles do not coincide for BC and vG soil models. This result suggests that when BC or vG soil models are used, σ_h^2 of steady state flow depends on the mean pressure head even if only f is considered as a stochastic process. The different behavior between the Gardner soil models and the vG and BC soil models can also be explained noting that for Gardner soils under unit gradient conditions, i.e.,

$$h = \frac{1}{\alpha_G} (\log q - \log K_S); \quad (13)$$

the derivative of h with respect to $\log K_S$ is independent of the prescribed flux, q , and hence of the mean pressure head. So the perturbation of the pressure head under these conditions does not depend on the perturbation of $\log K_S$. On the other hand, the derivative of the pressure head with respect to $\log K_S$ for unit gradient distribution in vG or BC soils depends on the prescribed flux and hence on the mean pressure head value.

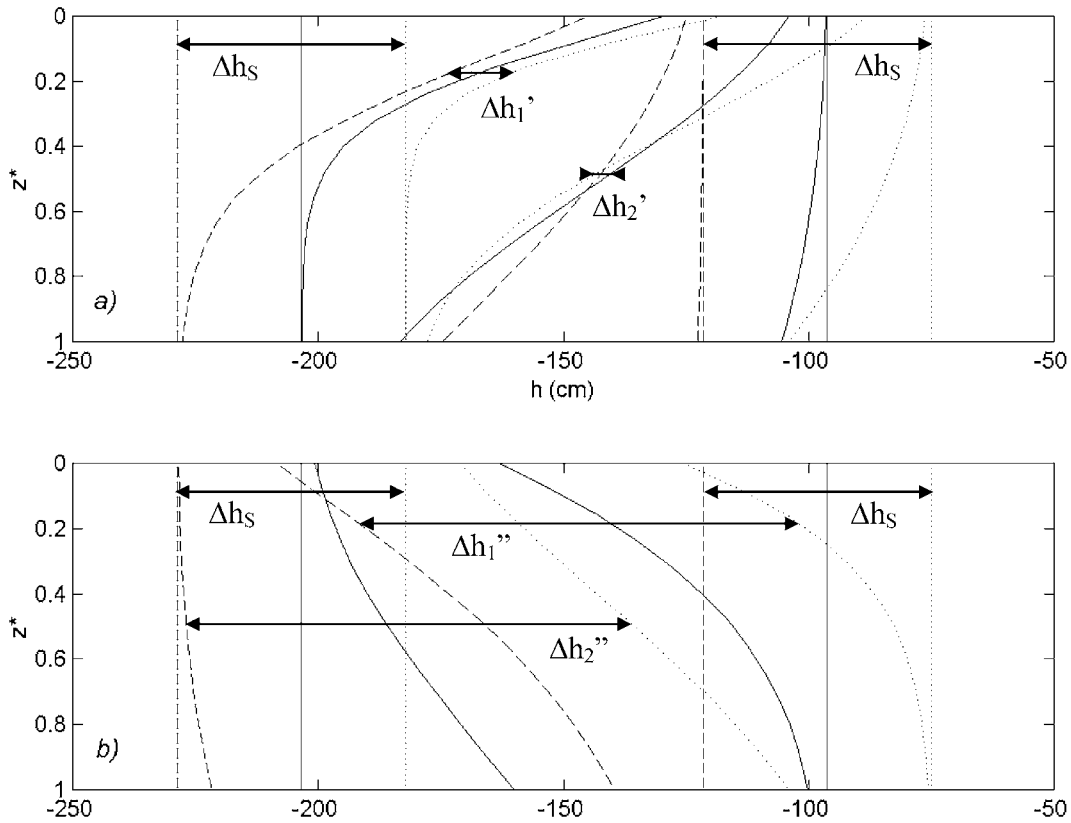


Figure 5. (a) Drying and (b) wetting front propagation in three GE soils with $K_{S1} < K_{S2} < K_{S3}$. Dashed, solid, and dotted curves refer to soils 1, 2, and 3, respectively.

[18] In Figure 4a, mean head profiles at different times are shown for the wetting scenario; the flux boundary condition at the surface is suddenly increased. Comparing Figure 4a with Figure 3a, differences in front propagation velocity and diffusive front are evident between the soil models. While the GE model in this case shows a smaller diffusive front than all other models, its diffusive front and velocity of the front do not depend on wetting or drying process [Srivastava and Yeh, 1991]. Initial and final steady state profiles for the three soil models GE, GL, and GR coincide with those for the drying case.

[19] The smaller diffusivity of the wetting process results in higher spatial gradients of pressure head and hence narrows the diffusive zone where transient process takes place. As a result, pressure head variance “waves” shown in Figures 4b and 4c are narrower than those for the wetting case. Pressure head variance peaks are still at the location where the highest mean pressure head gradient exists.

[20] Also, Figures 4b and 4c show that some reduction of the head variance comparing with the initial steady state conditions at the early time. To explain this behavior, in Figure 5a the head profiles are shown for a wetting front propagating in three GE soils, differing from each other only in K_S values ($K_{S1} < K_{S2} < K_{S3}$, where 1, 2, and 3 are the soil number). The wetting front is originated by the same sudden change in the constant flux boundary condition at the surface, as in Figure 4. The initial unit gradient pressure head values are evaluated by (13) and $h_1 > h_2 > h_3$. Once the flux boundary condition is increased, the wetting front propagation starts in the upper part of the three soils with different slopes: the larger the K_S value, the lower the initial pressure head value and the steeper and faster the wetting front. As a result,

differences in the pressure head values close to the surface tend to decrease at early times, from Δh_s to $\Delta h_1'$, and $\Delta h_2'$, or, in other words, the uncertainty in the pressure head value at these times decreases. After a while, differences in the pressure head profiles start to increase. The drying front propagation in the same soils is shown in Figure 5b. Differences in head values tend to increase also at early times, from Δh_s to $\Delta h_1''$ and $\Delta h_2''$, because the differences in pressure head values are not affected by differences in the drying front propagation velocity and diffusivity.

[21] Mean pressure head profiles, originated by a sudden change in the constant pressure head condition at the top boundary, are identical to those in Figure 3a, where the prescribed flux boundary condition is used, because of the way the prescribed head condition is defined. Pressure head variances are shown in Figures 6a and 6b. The prescribed head boundary conditions at the surface and at the water table yield a zero pressure head variance at the top and bottom boundaries. In the remaining part of the domain, far from the boundaries, the magnitudes of head variance of steady state profiles in Figures 6a and 6b are also different from those in Figures 3b and 3c. Such differences can be attributed to the random flux due to the stochastic nature of f and the prescribed head boundary condition. As for Figures 3b and 3c, the peaks of the pressure head variance under transient conditions are found at the locations of the maximum head gradient, and their values usually increase with time.

5. Conclusions

[22] A numerical model is applied to investigate an unsaturated front propagation in a bounded heterogeneous domain. The

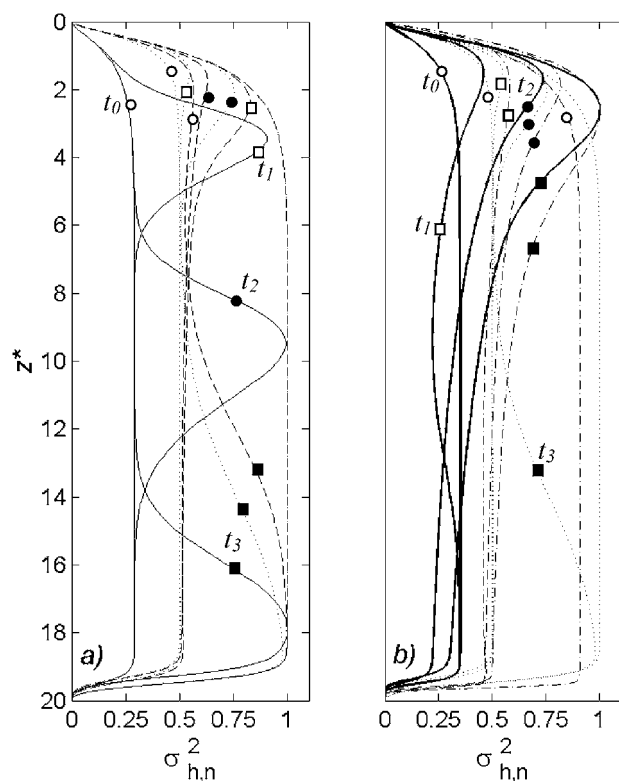


Figure 6. (a and b) Normalized pressure head variance profiles for GE (solid bold curves), GL (dotted curves), GR (dashed curves), vG (dashed-dotted curves), and BC (solid thin curves) soil models for a drying scenario and a constant head top boundary condition.

numerical model, unlike the spectral method and other analytical methods, allows investigation of the effects of different boundary conditions and soil models on pressure head variance profiles.

[23] In spite of the many advantages of the numerical approach we have to emphasize that it is based on a first-order approximation. For unsaturated flow problems, first-order approximation is valid if the unsaturated hydraulic conductivity variance is much less than one [Harter and Yeh, 1996]. Nevertheless, application of the first-order numerical model to the analysis of propagation of head variance yields some interesting results.

[24] Results of our analysis show that there is a strong proportionality of pressure head variance and pressure head gradient during transient flow when f is a stochastic variable. The constant flux boundary condition affects the pressure head variance distribution close to the surface, resulting in a decrease of the values at early times during wetting scenarios. On the other hand, a constant head boundary condition controls the variance profiles, under both transient and steady conditions, even far from the boundary.

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