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An Efficient Method for Simulating Steady Unsaturated Flow in Random Porous Media: Using an Analytical Perturbation Solution as Initial Guess to a Numerical Model

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Numerical simulation of flow through multidimensional heterogeneous soils under unsaturated conditions is a computationally intensive task. The governing unsaturated flow equation is nonlinear. The degree of nonlinearity depends on the unsaturated hydraulic properties of the soil and the degree of heterogeneity. In this paper, we present a highly efficient method to simulate unsaturated steady state flow through random porous media. Our method utilizes the analytical (approximate) solution derived by a perturbation-spectral method as an initial guess solution for a numerical model to simulate two-dimensional vertical infiltration problems. It is found that this approach, which we call "ASIGNing," reduces the required CPU time by one to two orders of magnitude. ASIGNing is demonstrated to operate successfully under a wide variety of boundary conditions which may substantially deviate from those imposed on the initial guess solution. A large range of mean and variances in the independent variables $\ln K_s$ and α or alternatively $\ln \alpha$ has been tested and it is shown that the method works well for variances of the unsaturated hydraulic conductivity $\sigma^2_{\ln K} \leq 5$ and average $\langle \alpha \rangle \leq 0.1$ [cm^{-1}].

INTRODUCTION

Effects of soil heterogeneity have been the focus of both field and theoretical research for the past decade [e.g., *Hills et al.*, 1991; *Hopmans et al.*, 1988; *Mantoglou and Gelhar*, 1987; *McCord et al.*, 1991; *Russo*, 1991; *Ünlü et al.*, 1990; *Wierenga et al.*, 1991; *Yeh et al.*, 1985*a*, *b*; *Yeh et al.*, 1986]. Analytical models are essential tools for investigating the effect of heterogeneity on flow and transport in the unsaturated zone. However, the nonlinearity of the governing flow equation, the degree of nonlinearity, and the spatial variability in the unsaturated hydraulic properties often prohibit the development of analytical solutions. Analytical solutions are only available for some special cases, such as one-dimensional steady state and transient infiltration in layered soil with Gardner type unsaturated properties [*Yeh*, 1989; *Warrick and Yeh*, 1990; *Srivastava and Yeh*, 1991]. For more general problems we often rely on numerical techniques such as finite difference and finite element methods [compare *Fletcher*, 1988; *Anderson and Woessner*, 1992].

The finite element or finite difference equations for unsaturated media are commonly written in form of a linearized matrix equation such as

$$\mathbf{A}(\mathbf{x}^m)\mathbf{x}^{m+1} = \mathbf{b} \tag{1}$$

where m indicates the outer, nonlinear iteration level, $\mathbf{A}$ is the coefficient matrix, $\mathbf{x}$ is the vector of unknown values, and $\mathbf{b}$ is the vector of known terms. Direct (noniterative) or indirect (iterative) methods are used to solve the inner, linear part of (1) numerically. In general, direct algorithms require a large amount of computer storage for multidimensional problems. Hence most numerical techniques employ so-called indirect or iterative methods for solving the linear part of (1) to improve CPU efficiency and to reduce the memory requirements for the computer.

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The nonlinear solution is essentially found by repeating the linear solution to (1) at increasing iteration levels m until the convergence criterion $|\mathbf{x}^{m+1} - \mathbf{x}^m| < \delta$ (a prescribed tolerance) is met. Several techniques have been developed based on (1) such as the Picard method and the Newton-Raphson method [*Ortega and Rheinbolt*, 1970].

If (1) represents a transient problem, both the inner and outer iteration procedure start from the initial conditions of the boundary value problem and march through time. For a steady state problem, the iterative procedure requires a starting approximate solution $\mathbf{x}^1$ (initial guess or initial solution). The initial guess has little bearing on the final solution. However, it can reduce the number of iterations that are necessary for convergence of the solution if the guess solution is close to the actual solution. In the case of nonlinear equations, no guarantee exists, even under the absence of round-off errors, that the outer or nonlinear iteration methods will converge under some predefined conditions. In general, the initial guess must therefore be close to the solution to avoid divergence of the outer iteration scheme. The degree of similarity between initial and actual solution that is required for convergence depends on the degree of heterogeneity and nonlinearity in the boundary value problem.

It is our experience that the numerical analysis of nonlinear, steady perturbation problems with either the Picard or the Newton-Raphson method is mostly impossible, since it is difficult to prescribe an initial guess that consistently leads to convergence in the solution of (1). One may circumvent this difficulty by using either a transient time-marching approach (i.e., solving the steady state flow problem by the transient approach) or a pseudo transient approach [*Fletcher*, 1988]. Both techniques diagnolize the matrix and expand the radius of convergence but they require numerous time steps to obtain an approximate steady state solution. As a result, such approaches often require large amounts of CPU time [e.g., *Ababou*, 1988]. In the past, convergence problems and CPU time requirements severely limited the numerical in-

vestigation of the effects of soil heterogeneity on unsaturated flow and transport. While numerical methods have enjoyed relatively widespread use for saturated problems, numerical stochastic analysis of unsaturated flow and transport has been an exercise with very limited applications.

To alleviate these problems, we suggest here that a very powerful initial guess can be provided by solving an approximate problem to which the analytical solution is known (to ASIGN: to use an analytical (or approximate) solution as initial guess to the numerical solver). In this paper, we develop a new technique which utilizes a spectral solution for flow in random porous media under unsaturated conditions as an initial guess solution for the Newton-Raphson iterative scheme in a numerical model. We demonstrate the advantage of the approach through several examples.

Statement of the Boundary Value Problem

Flow in two-dimensional heterogeneous porous media under fully unsaturated conditions is generally described by the Richards equation:

$$\frac{\partial}{\partial x_i}\left[K(h)\frac{\partial(x_1+h)}{\partial x_i}\right]=C(h)\frac{\partial h}{\partial t}\qquad i=1,\ 2\qquad (2a)$$

where x_1 and x_2 are the vertical and horizontal coordinates, respectively, and x_1 is positive upward, h is the matric potential (negative for unsaturated condition), and $K(h)$ is the unsaturated hydraulic conductivity, which is a function of h. The moisture capacity term $C(h) = d\theta/dh$ also varies with h. Under steady state conditions the right-hand side of (2a) vanishes and the solution becomes independent of the water retention function $\theta(h)$:

$$\frac{\partial}{\partial x_i}\left[K(h)\frac{\partial(x_1+h)}{\partial x_i}\right]=0\qquad i=1,\ 2\qquad (2b)$$

The parameteric relationship used in this analysis to describe $K(h)$ is an exponential model first suggested by *Gardner* [1958]. That is,

$$K(h)=K_s\exp(\alpha h)\qquad (3)$$

where K_s is the saturated hydraulic conductivity and α is a soil parameter defining the rate of reduction in $K(h)$ as a function of head h and hence defining also the degree of nonlinearity in (2). For transient solutions of (2a), the moisture release curve is given in the form suggested by *Russo* [1988] and is consistent with the pore model by *Mualem* [1976]:

$$\theta=\theta_r+(\theta_s-\theta_r)[e^{-0.5\alpha|h|}(1+0.5\alpha|h|)]^{2/(m+2)}\qquad (4)$$

where θ is the moisture content, θ_s is the moisture content at saturation, and θ_r is residual moisture content. Here m is a parameter commonly determined by fitting (4) to measured water retention curves. It accounts for the tortuosity of the flow path and the correlation between pores. For heterogeneous soils, K_s, α, m, θ_s, and θ_r may be functions of location. Equations (2)–(4) can be solved by either finite difference or finite element methods. In the following analysis, a Galerkin finite element model, MMOC2 [*Yeh et al.*, 1993], solves (2)–(4) with associated boundary conditions. MMOC2 solves the algebraic equation (1) resulting from finite element approximation of (2) using a preconditioned conjugate gradient solver on the inner level. The computer program implements the Newton-Raphson iteration technique to resolve the nonlinearity of the matrix equation at the outer iteration level. MMOC2 can be used to solve the steady state solution of (2b) either directly or via a transient solution of (2a) for $t\to\infty$, whereby the choice of $C(h)$ is arbitrary and can be made to improve the CPU efficiency (pseudo transient method). Since there is a trade-off between the choice of $C(h)$ and the size of the time step Δt, CPU time improvements due to an optimal choice of $C(h)$ are limited.

Formulation of the Initial Guess Solution

To obtain a close initial guess solution for steady state infiltration into heterogeneous porous media, where K_s and α in (3) are second-order stationary stochastic processes, a quasi-analytical solution based on a first-order perturbation analysis similar to the work by *Bakr et al.* [1978], *Gelhar and Axness* [1983], and *Yeh et al.* [1985a, b] is developed. Equation (2b) can be rewritten as

$$\frac{\partial^2 h}{\partial x_i}+\frac{\partial \ln K(h)}{\partial x_i}\frac{\partial h}{\partial x_i}+\frac{\partial \ln K(h)}{\partial x_1}=0\qquad (5)$$

where $i = 1, 2$. We use the perturbation notation for the random variables $\ln K_s$, α, and h:

$$\begin{aligned}\ln K_s &= F+f'\\ \alpha &= A+a'\\ h &= H+h'\end{aligned}\qquad (6)$$

where F, A, and H are the expected values of $\ln K_s$, α, and h, respectively, and f', a', and h' in zero-mean, second-order stationary perturbations. The unsaturated hydraulic conductivity is then given by

$$\ln K(h)=\ln K_s+\alpha h=F+f'+(A+a')(H+h')\qquad (7)$$

Using (6) and (7) in (5), expanding, subtracting the mean equation, neglecting all higher-order perturbation products, and assuming that the mean flow is in x_1 direction under unit mean gradient conditions (gravity flow), we arrive at the first-order perturbation approximation for the Richards equation:

$$\frac{\partial^2 h'}{\partial x_i^2}+A\frac{\partial h'}{\partial x_1}+H\frac{\partial a'}{\partial x_1}+\frac{\partial f'}{\partial x_1}=0\qquad i=1,\ 2\qquad (8)$$

Note that this is a linear equation. The linearization has been achieved by dropping the higher-order perturbation products and by assuming that the average gradient is unity. This equation can be solved numerically using a finite difference or finite element method for given heterogeneous a' and f' fields. The approximate solution will be much easier to obtain than that of (2b), since the problem has been linearized. Alternatively, if the porous medium is assumed to be of infinite extent and since a', f', and h' are stochastic stationary processes, one can solve (8) using a combination of spectral analysis and fast Fourier transform technique. A similar approach was successfully applied to horizontal saturated flow [*Gutjahr et al.*, 1992]. The continuous parameter stationary processes are represented by Fourier-Stieltjes integrals [compare *Priestley*, 1981]:

$$a'(\mathbf{x}) = \int_{-\infty}^{\infty} e^{i\mathbf{k}\cdot\mathbf{x}}\, dZ_{a'}(\mathbf{x})$$

$$f'(\mathbf{x}) = \int_{-\infty}^{\infty} e^{i\mathbf{k}\cdot\mathbf{x}}\, dZ_{f'}(\mathbf{k}) \qquad (9)$$

$$h'(\mathbf{x}) = \int_{-\infty}^{\infty} e^{i\mathbf{k}\cdot\mathbf{x}}\, dZ_{h'}(\mathbf{k})$$

where $dZ_p(\mathbf{k})$ are orthogonal complex stochastic processes, $p = f'$, a', or h'. The process $dZ_p(\mathbf{k})$ is a zero-mean univariate Gaussian random variable with a variance equal to the spectral density $S_{pp}(\mathbf{k})d\mathbf{k}$, which is the Fourier transform of the covariance function for the spatial random processes f', a', or h'. Any $dZ_p(\mathbf{k}_i)$ is statistically independent of $dZ_p(\mathbf{k}_j)$ for $i \neq j$. Using (9) in (8), a closed-form expression for the relationship between Fourier amplitudes of a', f', and h' can be obtained:

$$dZ_{h'}(\mathbf{k}) = \frac{ik_1(dZ_{f'}(\mathbf{k}) + H\, dZ_{a'}(\mathbf{k}))}{(k_1^2 + k_2^2 - iAk_1)} \qquad (10)$$

where $dZ_{a'}(\mathbf{k})$ may be assumed equal $\zeta dZ_{f'}(\mathbf{k})$ (i.e., a' and f' are perfectly correlated through $a' = \zeta f'$, where ζ is a proportionality constant); $dZ_{a'}(\mathbf{k})$ may also be chosen to be partially correlated to $dZ_{f'}(\mathbf{k})$ or independent. The $dZ_{f'}(\mathbf{k})$ and $dZ_{a'}(\mathbf{k})$ processes are generated as discretized, truncated spectral fields of $(2m)^2$ uncorrelated complex random numbers, where at each discretized spectral location k_{jl}, $0 < j \leq m$, $-m < 1 \leq m$ [*Gutjahr et al.*, 1992]:

$$dZ_p(k_{jl}) = (c_{jl} + id_{jl})(S_{pp}(k_{jl})\Delta k_1 \Delta k_2)^{1/2} \qquad (11)$$

c_{jl} and d_{jl} are independent normal random variables with zero mean and a variance of one half. To ensure that the spatial random processes p are real, we set $dZ_p(k_{-jl}) = dZ_p^*(k_{jl})$, the conjugate complex of $dZ_p(k_{jl})$; $dZ_{h'}(k_{jl})$ can then be computed explicitly (without solving a partial differential equation) using (10). The spatial solution h'_{jl} and the random input fields f'_{jl} and a'_{jl}, $0 < j, l \leq m$ are obtained after a numerical inverse fast Fourier transform (FFT) of their respective discretized spectral representations [*Gutjahr et al.*, 1992]. The two-dimensional spatial random field with m^2 points is only one quarter of the size of the inverse FFT of dZ_p due to the truncation of the spectrum and the resulting symmetry in the transformed field.

Recent field data indicate that the soil texture parameter α is lognormal distributed [e.g., *White and Sully*, 1992]. A first-order perturbation equation can be derived for this case as well. Following the approach by *Ababou* [1991], we write

$$\ln \alpha = G + \gamma'$$

$$\alpha = \exp(G + \gamma') = \Gamma \exp(\gamma') \qquad (12)$$

where $G = E[\ln \alpha]$ and γ' is a multivariate normal distributed random varible. Again using the first-order approximation, we can write α:

$$\alpha \approx \Gamma(1 + \gamma') \qquad (13)$$

Using (13) instead of the second equation in (6) for the otherwise identical derivation of the perturbation equation, the first-order perturbation equation in the case of lognormally distributed α becomes

$$\frac{\partial^2 h'}{\partial x_i^2} + \Gamma \frac{\partial h'}{\partial x_1} + H\Gamma \frac{\partial \gamma'}{\partial x_1} + \frac{\partial f'}{\partial x_1} = 0 \qquad i = 1, 2 \qquad (14)$$

From this, a quasi-analytical spectral solution algorithm is derived similar to the solution of (10):

$$dZ_{h'}(\mathbf{k}) = \frac{ik_1(dZ_{f'}(\mathbf{k}) + H\Gamma\, dZ_{\gamma'}(\mathbf{k}))}{(k_1^2 + k_2^2 - i\Gamma k_1)} \qquad (15)$$

which may then be utilized as initial guess to the numerical solution of (2) if α is a lognormal random variable (12).

TABLE 1. Parameters for the Numerical Experiments

	α Case(1) and ln α Case	α Case(2)
Mean ln K_s, cm/day	3.5	1.5
Variance $\sigma_{f'}^2$	0.1, 1.5, 6.0	1.5
Mean α: A, 1/cm	0.01	0.001
$\zeta_{a'f'} = \sigma_{a'}/\sigma_{f'}$	0.001	0.0002
Mean ln α: Γ, 1/cm	−4.6	···
$\zeta_{\gamma'f'} = \sigma_{\gamma'}/\sigma_{f'}$	0.1	···
Mean head H, cm	−150	−150

EXAMPLE PROBLEMS

To investigate the capability of ASIGNing at various degrees of soil variability and to compare the efficiency of the ASIGNed steady state solution with the hitherto standard (pseudo) transient numerical solution method we chose a principal parameter set that allowed variations in the moments of ln K_s, α, and ln α over several orders of magnitude. The values of both the deterministic and the stochastic parameters are summarized in Table 1. Our examples are for two-dimensional cross sections of 64 elements width and 64 elements depth. The size of the elements is 10 cm by 10 cm, resulting in a total domain size of 6.4 m by 6.4 m. In all simulations an exponential isotropic covariance function is specified to characterize the random variables f', a', and γ':

$$\text{Cov}(\mathbf{b}) = \sigma^2 \exp\left(\frac{|\mathbf{b}|}{\lambda}\right) \qquad (16)$$

where σ^2 is the variance of the random variable, $\mathbf{b}$ is the separation distance, and $\lambda = 50$ cm is the correlation length.

The mean of α, A, determines the degree of nonlinearity in (2). Initially, two values are chosen for A: 0.01 cm^{-1}, which is typical for fine sandy to loamy soils (α case (1)), and 0.001 cm^{-1}, which is typical for fine-grained silty and clay rich loamy soils (α case (2)). We use the α case (1) to investigate the effect of different boundary conditions. The α case (2) and the ln α case are used to demonstrate the efficiency and flexibility of the method with respect to various possible applications.

The boundary conditions are (1) of the Dirichlet type (prescribed head) on all boundaries; (2) of the Dirichlet type at the top and bottom of the domain, but with zero flux on the vertical boundaries; (3) of the Dirichlet type at the bottom boundary, zero flux at the vertical boundaries, and a prescribed flux of $q = 7.4$ cm/hour at the top boundary (then

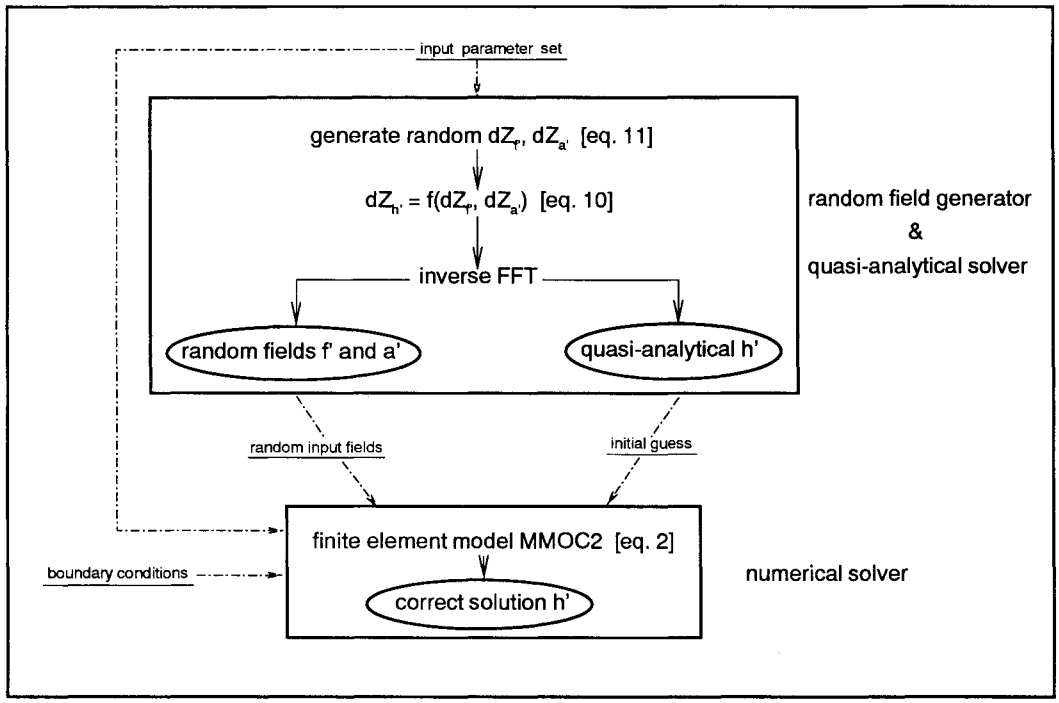

Fig. 1. Schematic overview of ASIGNing.

$H \approx -150$ cm); (4) unit gradient conditions at the bottom boundary, zero flux at the vertical boundaries and prescribed flux $q = 7.4$ cm/hour at the top boundary; (5) water table boundary at the bottom (uniform Dirichlet, $h_{BC} = 0$), all other boundaries are Dirichlet boundaries; (6) water table boundary at the bottom (uniform Dirichlet, $h_{BC} = 0$), zero flux at the vertical boundaries and Dirichlet boundary at the top; and (7) the ln α case is tested with boundary condition 1 and parameters similar to the α case (1) (see Table 1).

For the combined ASIGNing method each Dirichlet boundary (except the water table condition) is equal to the perturbed random head boundary produced by the quasi-analytical solution for an infinite domain. In the transient solutions all head boundaries are uniformly set to $H = -150$ cm, which is the mean head used for all example problems. All of the above boundary value cases are run at variances $\sigma_{f'}^2 = 0.1$, 1.5, and 6. Some cases are also repeated at $\sigma_{f'}^2 = 0.01$, 0.5, 1.0, and 3.0. The geometric mean of K_s is 33.1 cm/hour in α case (1) and 4.5 cm/h in α case (2); a' and γ' are assumed to be correlated to ln K_s with proportionality constants $\xi = 0.001$ and 0.1, respectively. It is chosen such that none or only minor portions of the domain become saturated, even at large matric potential variances. Partial saturation poses no computational problem to the numerical code MMOC2, but our interest focuses on unsaturated conditions. We also repeat the α case (1) with $\sigma_{f'}^2 = 1.5$ for domain sizes ranging from 32^2 to 256^2 elements to demonstrate the applicability of ASIGNing to small as well as large numerical grids. All simulations are performed twice: one simulation with the transient approach using the transient option of MMOC2 and one simulation with the ASIGNing method, which combines the quasi-analytical solver with the steady state version of MMOC2. Except for the boundary conditions, all deterministic and stochastic parameters and the constitutive equations for $K(h)$ and $\theta(h)$ are identical for the analytical, the steady state, and the transient solutions of each example problem. The random fields of f' and a' or γ' produced to obtain the initial guess via (10) or (15), respectively, are used as random field input to the steady state and transient numerical solutions. A schematic overview of the ASIGNing methodology is given in Figure 1.

Results and Discussion

The Quasi-Analytical, the ASIGNed, and the Transient Numerical Solution in Comparison

It is generally known that the first-order perturbation equation (8) is a valid approximation to the nonlinear Richards equation (2*b*) for variances of $f' \ll 1.0$ [*Yeh et al.*, 1985*a*]. Hence for problems involving only small perturbations, the quasi-analytical spectral solution technique itself is expected to be satisfactory. Figure 2 shows that the head field from the quasi-analytical spectral solution to (8) is, indeed, in very good agreement with the ASIGNed solution to (2*b*) at $\sigma_{f'}^2 = 0.1$. At higher variances, the approximate solution deviates significantly from the "true" (numerical) solution of the Richards equation, in particular with respect to the head gradients. *Harter et al.* [1992] showed that the velocity fields derived from the quasi-analytical head solution to (8) are not divergence-free (i.e., not without artificial sources and sinks) for $\sigma_{f'}^2 > 0.25$. In contrast, the numerical solution implicitly guarantees a mass-balanced head distribution which will result in a divergence-free velocity field. It is the inaccuracy in the head gradient field which prevents the spectral solution to (8) to be a useful tool for transport simulations in highly variable media. Nevertheless, the overall spatial head distribution pattern is well preserved by the quasi-analytical spectral solution to (8), even at large variances (Figure 3). This may explain why the quasi-

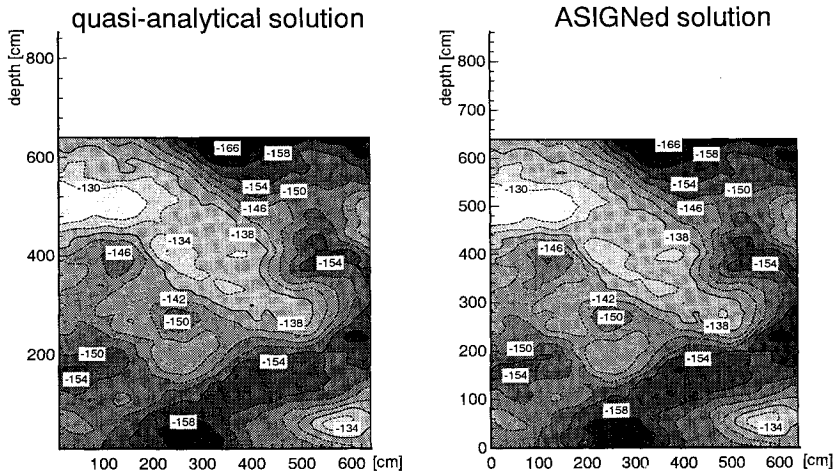

Fig. 2. Low variability: comparison of the first-order perturbation solution obtained by the quasi-analytical spectral method with the ASIGNed finite element solution to the Richards equation under boundary condition 1 at $\sigma_f^2 = 0.1$. The labels indicate the head (centimeters) at the nearest contour line.

analytical solution provides an initial guess which allows a direct numerical steady state solution of (2) much beyond the usual limits of the first-order perturbation approach.

With regard to solution uniqueness, we find throughout the set of experiments performed that the ASIGNed solutions are in excellent agreement with the those obtained by the time-marching approach. As an example, Figure 4 compares the ASIGNed with the late transient solution for α case (1) under boundary conditions (3) at $\sigma_f^2 = 6.0$. The only differences in the two solutions are near the bottom of the domain due to different constant head boundary conditions: the ASIGNed solution has a random head boundary given by the initial guess. The transient approach is based on a uniform head boundary condition with $h = -150$ cm. Given the agreement between the two solutions for the entire range of cases tested, we conclude that the ASIGNed solutions are as exact as the late time transient numerical solutions to (2).

Efficiency of the ASIGNed Solutions

The experiments show that the quasi-analytical spectral solution method to (8) is an extremely CPU-efficient algorithm to obtain approximate solutions to (2*b*) (Figure 5). Due to its spectral nature the number of computational steps is finite and independent of σ_f^2. The savings in CPU time over the transient time-marching numerical solution of (2*a*) is on the order of three magnitudes and more: the quasi-analytical solution of (8) on a discretized grid of 64 × 64 points takes less than 1 s on an IBM RS6000/560 workstation, while the CPU time of the transient finite element solution with 64 × 64 elements is on the order of tens of minutes for $\sigma_f^2 = 0.1$ (for a comparison of the performance of the IBM RS6000/560, see *Tripathi and Yeh* [1993]).

At higher variances numerical solutions must be sought to correctly solve Richards equation (2) and the main purpose

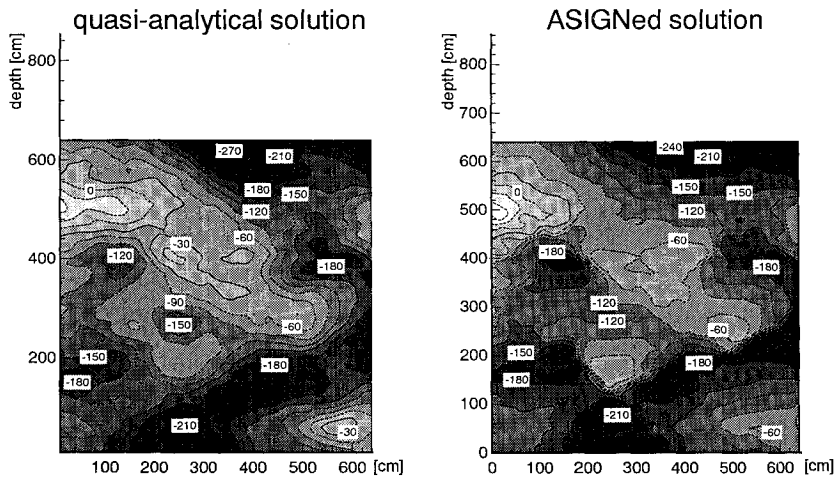

Fig. 3. High variability: comparison of the first-order perturbation solution obtained by the quasi-analytical spectral method with the ASIGNed finite element solution to the Richards equation under boundary condition 1 at $\sigma_f^2 = 6.0$. The labels indicate the head (centimeters) at the nearest contour line.

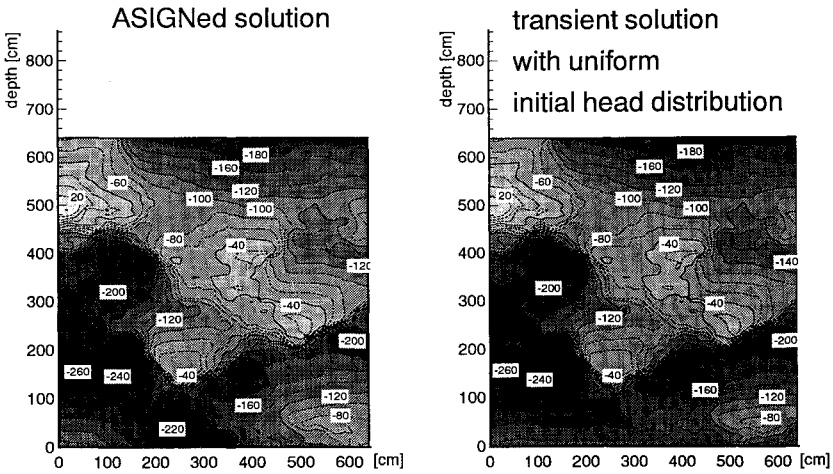

Fig. 4. Boundary condition 3 with three flux type boundaries: comparison of the ASIGNed steady state finite element solution to the Richards equation with that obtained by transient time marching at $\sigma_f^2 = 6.0$. The labels indicate the head (centimeters) at the nearest contour line.

of ASIGNing is to reduce the CPU time requirements of the numerical solution. Indeed, the CPU time savings of the combined approach (ASIGNing) over the transient simulation technique are of a factor 20–30 at any input variance (Figure 5). The computation time of the initial guess (1.5 s of which almost 1 s is input/output) is almost negligible compared to the ASIGNed numerical solution time.

While the first example in Figure 5 contrasts two technically identical problems, since both the ASIGNed steady state and the transient solutions are subject to Dirichlet boundary conditions, the physical problems solved are different: the transient solution assumes a uniform head of −150 cm all around its domain. The assumption of such uniform head boundaries is difficult, since in most unsaturated flow and transport applications little is actually known about the head boundaries of the domain. The ASIGNed steady state solution, however, takes advantage of the random head boundaries provided by the initial guess, thus solving for an approximate quasi-infinite domain. In practice, the use of random head boundaries provided by (10) or (15), which are (approximately) consistent with the random input parameter fields ln K_s and α, is much more realistic than uniform head boundaries. With the random boundary head approach one can simulate a soil domain that has no definite boundaries. Many authors have circumvented uniform Dirichlet boundaries by specifying flux boundaries

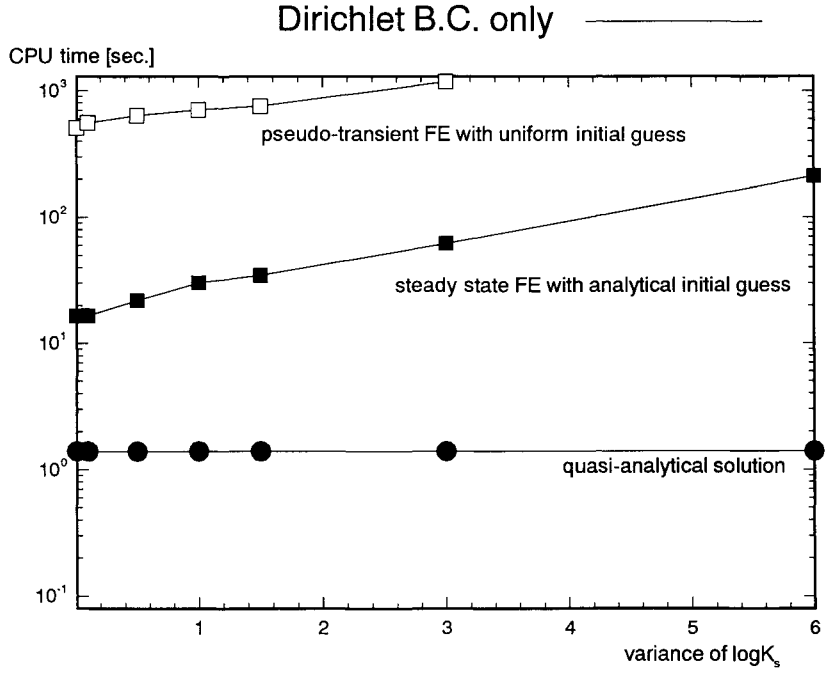

Fig. 5. CPU time (seconds) as a function of σ_f^2 for the quasi-analytical spectral method, the ASIGNed numerical solution (without computation of the initial guess), and the transient numerical solution with a uniform initial head distribution. The numerical cases are computed with boundary condition 1.

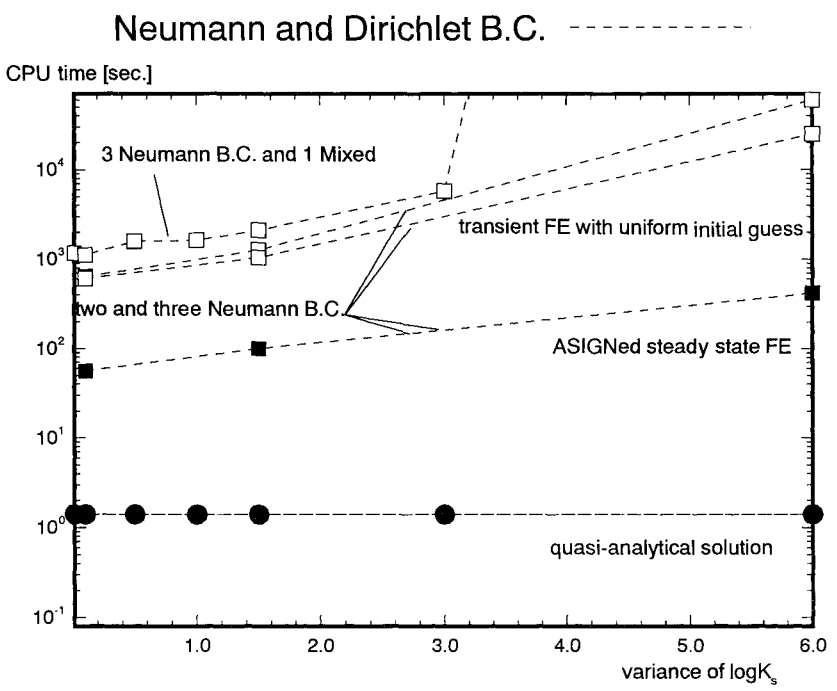

Fig. 6. CPU time (seconds) as a function of σ_f^2 for the quasi-analytical spectral method, the ASIGNed numerical solution (without computation of the initial guess), and the transient numerical solution with a uniform initial head distribution. The numerical cases are computed with boundary conditions 2 and 3. No convergence in the ASIGNed solution was achieved for boundary condition 4.

(Neumann conditions) around the domain, which are generally more CPU expensive to solve. The CPU savings of the combined approach with random Dirichlet conditions over the transient approach with at least three Neumann conditions are approximately two orders of magnitude (Figures 5 versus 6).

In the examples tested, both the ASIGNed steady state and the time-marching (transient) solutions cost increasing CPU time as more and more Neumann conditions are introduced. However, throughout the range of variability ASIGNing remains a much more efficient technique (Figure 6). Surprisingly perhaps, the most significant time savings (two orders of magnitude) under otherwise identical boundary conditions are obtained for the water table scenario with no-flow conditions on the vertical boundaries (Figure 7). The head field in this case is not only heterogeneous, but also deviates from the uniform mean head assumption implicit in the initial solution to (8). This shows the broad applicability of ASIGNing.

The only boundary conditions, for which no ASIGNed steady state solution is obtained are those which involve a unit gradient boundary condition at the bottom of the cross section. The unit gradient boundary is a Cauchy or mixed type condition. *Ünlü et al.* [1990] have shown for the one-dimensional case that unit gradient boundary conditions are associated with head variances that are higher than those associated with other types of boundary conditions, which may explain the convergence problems of ASIGNing in this case.

Figure 8 shows that the efficiency of our proposed method decreases only slightly as the size of the domain increases from 1,000 to over 65,000 elements. At any domain size, the proposed method is particularly powerful at high variances when compared to the traditional transient solution CPU time. The method also applies successfully to the ln α case. Table 2 provides some example CPU times for both the ln α case and for α case (2) with much smaller mean α. The efficiency of the method is comparable to the cases shown in Figure 5.

With regard to the overall efficiency of ASIGNing over the common transient method it should be noted that the convergence criteria of the transient method is not coded into the model (such as a stopping rule of the type Max $|h_{t+1} - h_t| < \delta$), since transient solutions may change very little within one time step without having necessarily reached steady state. Rather, the transient heads are continuously evaluated at seven points uniformly distributed over the domain. From this head record, the actual CPU time for the transient approach is determined retroactively. In practice, the pseudo transient approach may therefore require significantly more CPU time than indicated in Figures 5–8 and in Table 2, since the number of time steps required to approach steady state are generally not known ahead of the simulation.

Limitations of ASIGNing

The above examples have shown that ASIGNed solutions can be obtained over a wide range of variances. However, it must be emphasized that the success of the method is not unlimited due to the first-order character of the analytical solution. As was indicated before, terms of second and higher order that were neglected in deriving the perturbation equation (8) and (14) become significant at higher variances of f' and/or a'. Hence the (initial guess) solutions (10) and (15) deviate more strongly from the steady state solution to (2*b*) as the perturbations increase (compare Figures 2 and 3). Once the difference between the two solutions is larger than

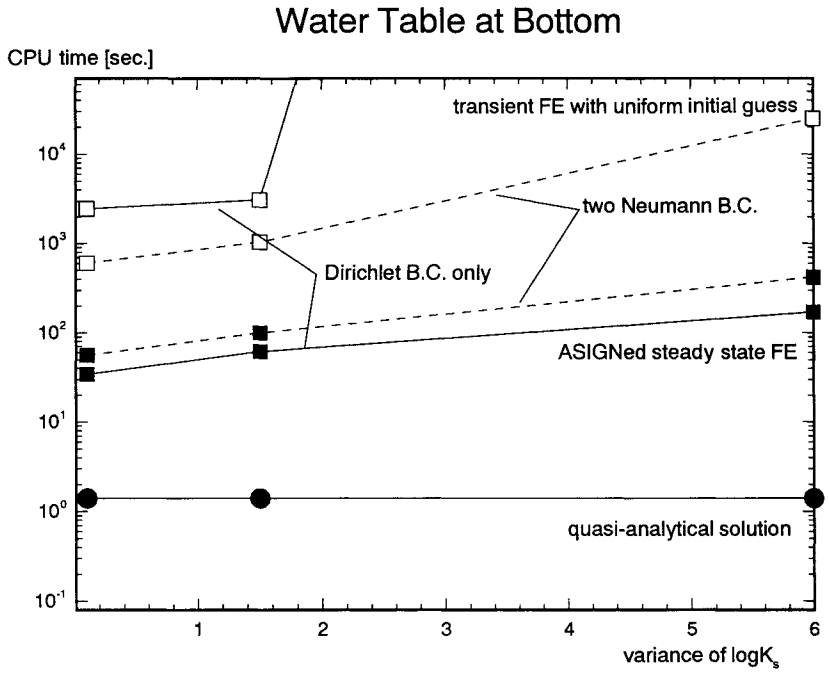

Fig. 7. CPU time (seconds) as a function of σ_f^2 for the quasi-analytical spectral method, the ASIGNed numerical solution (without computation of the initial guess), and the transient numerical solution. The numerical cases are computed with boundary conditions 5 and 6.

the convergence radius of the Newton-Raphson method, a direct steady state solution is impossible to obtain even with the quasi-analytical initial guess. Our experiences with the above examples have shown that ASIGNing is successful up to variances of 5 in the logarithm of the unsaturated hydraulic conductivity $\sigma^2_{\ln K'}$ with $A \leq 0.01$ [cm^{-1}] and $\sigma^2_{a'} \leq 0.006$. Since α determines the degree of nonlinearity, the mean and variance of α or ln α and its correlation to f' are expected to be critical to the success of ASIGNing.

To explore the limits of the method additional ASIGNed simulations are implemented with independent random parameters f', a', and γ' and a wider range of means and variances in α as before. First, the ln α case described above is repeated with independent parameters f' and γ'. The

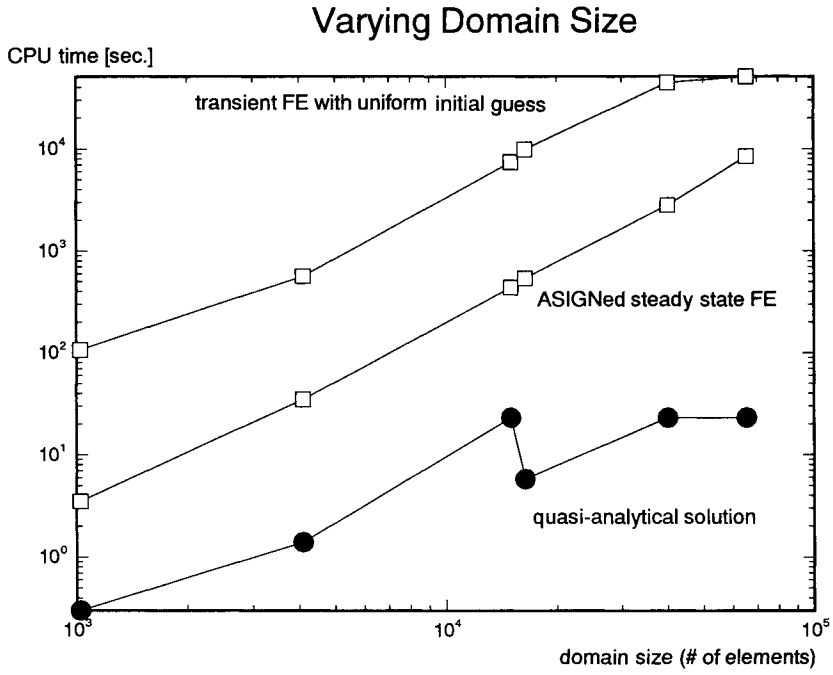

Fig. 8. CPU time (seconds) as a function of domain size: comparison of the quasi-analytical spectral method, the ASIGNed numerical solution (without computation of the initial guess), and the transient numerical solution. The numerical cases are computed with boundary conditions 1.

TABLE 2. Results of the α Case(2) and the ln α Case Experiments

	$\sigma^2_{f'}$ (Saturated Hydraulic condition)	$\sigma^2_{[\ln K]'}$ (Unsaturated Hydraulic Condition)	CPU Time, s (Pseudotransient)	CPU Time, s (Steady State With ASIGNing)
α Case(1)	0.1	0.062	559	16.6
α Case(1)	1.5	0.97	758	34.8
α Case(1)	6.0	4.05	N/A	211
α Case(2)	1.5	1.36	695	24.6
ln α Case	0.1	0.062	563	16.6
ln α Case	1.5	0.96	743	39.4
ln α Case	6.0	3.99	N/A	63.9

N/A, transient solution did not converge.

variances of the independent γ' in these cases are 1/100 of the variance $\sigma^2_{f'}$ specified, just as in the first ln α case with dependent random fields. The CPU times required for the two lower $\sigma^2_{f'}$ cases are 50% larger than those for the dependent case. Convergence is achieved except for the case of $\sigma^2_{f'} = 6.0$. In this independent ln α case, convergence is obtained with $\sigma^2_{f'} \leq 4.5$, which results in an unsaturated ln K variance $\sigma^2_{\ln K'} \leq 5$.

To separate the effects of f' and γ' at a given geometric mean $\langle\alpha\rangle_g = 0.01$ [cm^{-1}], we determined the largest $\sigma^2_{\gamma'}$ for which convergence is achieved at different $\sigma^2_{f'}$. At both $\sigma^2_{f'} = 0.1$ and 1.5 solutions are obtained if $\sigma^2_{\gamma'} \leq 0.5$, although the range in head variance for $\sigma^2_{\gamma'} = 0.5$ spans from 1470 cm^2 to 2300 cm^2, respectively, and the range of unsaturated hydraulic conductivity variances spans from 1.9 to 3.5, respectively. For $\sigma^2_{f'} = 4$, solutions are obtained with $\sigma^2_{\gamma'} \leq 0.2$. At even higher variances of $\sigma^2_{f'} = 4.7$, the maximum usable $\sigma^2_{\gamma'}$ reduces to 2×10^{-5}. Increasing the geometric mean of α to 0.1, which is typical of a coarse sand, shows that the variance of γ' is slightly more limited in applications with ASIGNing the ln α case. At variances $\sigma^2_{f'} = 1$, 5.3, and 7.4 the maximum usable $\sigma^2_{\gamma'}$ are 0.024, 0.01, and 0.0001, respectively, resulting in unsaturated hydraulic conductivity variances $\sigma^2_{\ln K'} = 3.0$, 4.0, and 4.2, respectively.

In the case of independent, normal distributed α where the first-order perturbation solution is not based on an approximation similar to (13), ASIGNing is also successful for a large range of $A = \langle\alpha\rangle$ without loss of CPU efficiency. At $\sigma^2_{f'} = 1.0$ and $A = 0.1$ [cm^{-1}], the largest possible $\sigma^2_{a'}$ is 0.01 ($\sigma^2_{\ln K'} = 2.0$, $\sigma^2_{h'} = 235$ cm^2), and at $A = 0.5$ [cm^{-1}] it is 0.007 ($\sigma^2_{\ln K'} = 0.77$, $\sigma^2_{h'} = 9$ cm^2). At smaller variances of a' and $A = 0.1$ [cm^{-1}] ASIGNed solutions are generally possible if $\sigma^2_{\ln K'} \leq 4.3$. These limits are obtained for the particular seed used to generate the random numbers c_{jl} and d_{jl} in (11). For other seeds the limits vary slightly and should therefore be taken as guidelines only.

The experiments show that three parameters seem to be most important to define the range of solutions for which ASIGNing is possible: the variance of the unsaturated hydraulic conductivity, the mean of α, and the variance of α, where the latter two parameters mainly identify the degree of nonlinearity in our problem (2). For the mean of $\alpha \leq 0.01$ or the mean of ln $\alpha \leq -4.6$, cases resulting in $\sigma^2_{\ln K'} \leq 4$ (or even 5) are solvable with ASIGNing as long as, for example, in the ln α case the variance of $\gamma' \leq 0.5$. At $\langle\alpha\rangle_g = 0.1$ and for a given $\sigma^2_{f'}$ ASIGNing is successful for $\sigma^2_{\gamma'}$ such that $\sigma^2_{\ln K'}$ does not exceed 4. The α case remains solvable for $\sigma^2_{a'} \leq 0.01$ at $A = 0.1$ [cm^{-1}]. These findings seem to be independent of the correlation between f' and a' or γ', independent of $\sigma^2_{f'}$ (so long as $\sigma^2_{\ln K'}$ does not exceed 3–4), and independent of the resulting head variance. At higher A the restrictions on the maximum conductivity variance are tighter, but overall the method has been shown to be successful for a broad range of parameters encountered under realistic field conditions.

Extensions of ASIGNing

It has already been emphasized that the boundary value problem for the initial guess, which is given by the analytical solutions (10) or (15), is different from the boundary value problems stated above for the numerical solver of (2). For all the above boundary value problems the analytical solution provides an initial guess based only on the assumption of an unbounded domain, while the numerical solutions are mathematically speaking all subject to bounded domain conditions. It is important to understand that the quasi-analytical solutions for all of the cases tested serve only as first approximations and are not a defining part of the numerical solution. The set of boundary conditions is intended to show the variety of boundary conditions, for which the single analytical solution (10) may successfully be used as initial guess such that the steady state finite element simulation of (2*b*) converges directly.

Theoretically, it is possible to generate quasi-analytical solutions to (8) not only with different boundary conditions than the numerical solutions to (2), but also with a different input set $\{F^*, \sigma^2_{f'}{}^*, A^*, \sigma^2_{a'}{}^*, H^*\}$ to better approximate the solution of (2) subject to the input parameter set $\{F, \sigma^2_{f'}, A, \sigma^2_{a'}, H\}$. This approach may be taken because the spectrally generated random fields of $\{f', a'\}$ and $\{f'^*, a'^*\}$ are identical in structure when different variances are specified, if the same seed is used for the spectral random field generator. Recall from (11) that $dZ_p(\mathbf{k})$, $p = f', a'$ are independent random numbers with a variance equal to $S_{pp}(\mathbf{k})d\mathbf{k}$. Since the spectral density function $S_{pp}(\mathbf{k})$ is the Fourier transform $\mathcal{F}$ of the covariance function (16), where σ^2_p is independent of location $\mathbf{x}$ or spectral wave number $\mathbf{k}$, it can easily be shown that the spectral density is a linear function of the variance σ^2_p:

$$S_{pp}(\mathbf{k}) = \sigma^2_p \mathcal{F}(\mathrm{Cor}_{pp}(\mathbf{b})) \tag{17}$$

where $\mathrm{Cor}_{pp}(\mathbf{b}) = \mathrm{Cov}_{pp}(\mathbf{b})/\sigma^2_p$ is the normalized correlation function. Then both $dZ_p(\mathbf{k})$ and their inverse fast Fourier transforms $f'(\mathbf{x})$ and $a'(\mathbf{x})$ are linearly dependent on σ^2_p. The quasi-analytical head solution h' will also produce identical

structures for different σ_p^2. They merely differ in the amount of excitation in their perturbed structure as shown by the quasi-analytical solutions in Figures 2 and 3. The same is not true for the head solution to (2*b*) due to its nonlinear character. Yet the structures are similar as shown by the ASIGNed head solution in Figure 2 produced from random fields of correlated f' and a' with $\sigma_{f'}^2 = 0.1$ and the ASIGNed head solution shown in Figure 3 which is based on random fields with $\sigma_{f'}^2 = 6.0$.

It is therefore conceivable to generate the initial guess solution with a meaningful, but arbitrary set of parameters $\{F^*, \sigma_{f'}^2{}^*, A^*, \sigma_{a'}^2{}^*, H^*\}$ to produce a certain structure in the initial head h', which is closer to the solution of (2) subject to $\{F, \sigma_{f'}^2, A, \sigma_{a'}^2, H\}$ than an initial head that is also based on $(F, \sigma_{f'}^2, A, \sigma_{a'}^2, H\}$. The practical procedure is then as follows: after obtaining the initial head h' with an arbitrary set $\{F^*, \sigma_{f'}^2{}^*, A^*, \sigma_{a'}^2{}^*, H^*\}$, one regenerates f' and a' with the same seed, but the input set $\{F, \sigma_{f'}^2, A, \sigma_{a'}^2, H\}$, and then procedes to solve the steady state numerical solution with the latter random fields of f' and a' but the former h' as initial guess. The water table problem α case (1) with the boundary condition 6 is a simple example of such an application: the initial head solution is based on a uniform mean head H^*; the numerical simulation solves a problem of vertically varying $H(z)$. The number of variations in this method is potentially endless and depends directly on the problem type. Further research is warranted, but it is beyond the scope of this paper to further investigate those possibilities.

In principle, ASIGNing can also be applied for cases where a solution to (2*b*) is sought with an unsaturated conductivity function $K(h)$ different from (3). In this case the parameters K_s and α in (3) have to be determined such that the head field from (10) is similar to that solving (2*b*) with the desired $K(h)$ function. A prominent example is the use of *Van Genuchten*'s [1980] constitutive relationships for $K(h)$ and $\theta(h)$ in the numerical solution of (2). While *Gardner*'s [1958] equation for $K(h)$ (3) is necessary for the derivation of (10), it is in many practical circumstances of rather limited use while Van Genuchten's $K(h)$ model has generally been more applicable to field soils. ASIGNing a Van Genuchten based solution to (2*b*) may be possible by defining equivalent parameters f' and a' for (10) analytically [*Russo et al.*, 1991]. This is cumbersome, however, since an equivalent f' and a' need to be determined for each random replicate of Van Genuchten parameters. Alternatively, the equivalent moments $\{F^*, \sigma_{f'}^2{}^*, A^*, \sigma_{a'}^2{}^*\}$ of the $K(h)$ parameters in (3) can be graphically matched by trial and error with those desired for the Van Genuchten $K(h)$: the parameter set $\{F^*, \sigma_{f'}^2{}^*, A^*, \sigma_{a'}^2{}^*\}$ is manually adjusted such that a random sample of Gardner's $K(h)$ curves best matches against a random sample plot of Van Genuchten's $K(h)$ curves. The latter approach may be time-consuming for a single simulation, and a transient solution is probably obtained faster. In most cases, however, ASIGNing will be used as part of a Monte Carlo simulation, and a single trial and error definition of a suitable parameter set for obtaining the initial guess may solve hundreds of Monte Carlo runs.

CONCLUSION

In many instances and particularly in the case of heterogeneous, steady, nonlinear problems, numerical solutions take prohibitive amounts of CPU time or lead to divergence in the iterative solution process. Typically, a uniform initial guess is provided by the user, even if the steady solution is nonuniform. For problems involving heterogeneous parameter fields, e.g., flow through variably permeable porous media, such an initial guess is generally so different from the solution that steady solution techniques fail and transient time-marching or pseudo transient methods must be employed, which are associated with high computation time.

For the large range of heterogeneous, unsaturated flow problems presented we developed a quasi-analytical spectral solution technique, which is a first-order linearized perturbation approximation to the governing nonlinear stochastic equation. This quasi-analytical solution is used as an initial guess solution in a finite element model which solves the nonlinear governing flow equation (2*b*) (analytical solution as initial guess to numerical solver (ASIGNing)). ASIGNing renders up to two orders of magnitude of CPU time savings. To our knowledge this is the first time stochastic analytical solutions have been combined with their respective numerical solutions. We have shown that the methods can successfully be applied to a wide range of field conditions with average α ranging from 0.001 [cm^{-1}] to 0.1 [cm^{-1}] and the variance of the log-unsaturated hydraulic conductivity being as large as 5. An even wider range of applications is conceivable once the parameters used to obtain the initial guess solutions are determined separately instead of using the identical set of parameters for both the initial guess and the numerical solution. ASIGNing works for correlated and uncorrelated f' and a' fields alike, and can be adopted to solve problems involving lognormal distributed α. The success of this particular combination of a quasi-analytical with a numerical method is very encouraging, since the nature of this technique is very general and many related problems in fluid dynamics may be solved similarly.

Another advantage of this particular approach is that random fields are generated intrinsically instead of separately. Furthermore, the first-order perturbation solution used here as initial guess allows to model vertical soil domains with random head boundaries thus eliminating boundary effects to the degree to which the first-order solution is accurate. Partial boundary conditions can alternatively be introduced through conditional simulation techniques, a possibility that is currently under research. CPU time enhancements of one and a half to two orders of magnitude allow for the first time the implementation of Monte Carlo techniques to solve unconditional and conditional stochastic unsaturated flow and transport problems (T. Harter, unpublished manuscript, 1993).

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