7. AN EFFICIENT METHOD FOR SIMULATING STEADY UNSATURATED FLOW IN RANDOM POROUS MEDIA: USING AN ANALYTICAL PERTURBATION SOLUTION AS INITIAL GUESS TO A NUMERICAL MODEL

7.1 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., 1985a,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 make the development of analytical solutions difficult. 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 one often relies on numerical techniques such as finite difference and finite element methods (c.f. 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:

$$\mathbf{A}(\mathbf{x}^{m})\mathbf{x}^{m+1} = \mathbf{b}(\mathbf{x}^{m}) \qquad (7\text{-}1)$$

where m indicates the outer, nonlinear iteration level, **A** is the linear coefficient matrix, **x** the vector of unknown values, and **b** the vector of known terms. Direct (non-iterative) 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. Hence, most numerical techniques employ so-called indirect or iterative methods for solving the linear part of eqn. (7-1) to improve CPU-efficiency and to reduce the memory-requirements for the computer.

The non-linear solution is essentially found by repeating the linear solution to (7-1) at increasing iteration levels m until the convergence criteria $|x^{m+1} - x^m| < \delta$ (a prescribed tolerance) is met. Several techniques have been developed based on (7-1) such as the Picard method and the Newton-Raphson method (Ortega and Rheinbolt, 1970).

If (7-1) were to represent a transient problem, both the inner and outer iteration procedure would start from the initial conditions of the boundary value problem and march through time . For a steady-state problem, the iterative procedure initially requires an approximate solution $\mathbf{x}^1$ (initial guess or initial solution). The initial guess has little bearing on the final solution. But it can reduce the number of iterations 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 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.

The solution of the perturbation flow problem (4-1b) for heterogeneous media 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 (7-1). 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) together with simple uniform or linearly varying initial solutions. Both techniques diagonalize the matrix and expand the radius of convergence but they require numerous time steps to obtain an approximate steady-state solution. In the solution of Richards equation (4-1a), a trade-off between the choice of C(h) and the size of the time-step Δt limits

options for CPU-time improvements, when the pseudo-transient method is used. As a result, such approaches often require large amounts of CPU time (chapter 6 in this work; Ababou, 1988, p.649, p.684, pp.681ff.). In the past, convergence problems and CPU time requirements often limited the investigation of the effect of heterogeneity in unsaturated soils. 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 (chapter 6). It is desirable to obtain the steady-state solution to (4-1b) without resorting to time-marching methods to improve CPU efficiency.

To alleviate the convergence and CPU time problems, it is suggested 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 chapter, it is demonstrated how the first order spectral solution can be used to provide such an initial guess to solve the 2-D steady-state Richards equation (4-1)b with Gardner's K(h) model (4-8) numerically in a very efficient manner. The advantage of the approach over the pseudo-transient approach utilized in chapter 6 is demonstrated through several examples.

7.2 Formulation of the Initial Guess Solution

In chapter 4, a first order perturbation solution to the steady-state Richards equation (4-1b) is developed based on spectral analysis. (4-26) gives the spectral solution of the steady-state head given the spectral representation of lognormally distributed input random fields of $\log K_s$ (log: natural logarithm) and α. The necessary random fields can be generated with any of the random field generators described in chapter 3. This requires a Fourier transform of the random fields of f' and a' to obtain $dZ_{f'}$ and $dZ_{a'}$ in (4-26). By generating the random fields with the SRFFT method, $dZ_{f'}$ and $dZ_{a'}$ are obtained directly by virtue of (3-3) and $dZ_{h'}$ is easily obtained by the explicit relationship provided in (4-26). Inverse FFTs are applied to each of

the three discrete z-fields representing f', a', and h' just like in the SRFFT random field generator (3-13). Not only has a set of input random fields f' and a' been generated; the approximate solution h' is also available. The f' and a' random fields are the input random fields for the numerical model, and h' is used as initial guess solution to the numerical solver. Only the use of the first order head solution as initial guess has allowed for obtaining steady-state solutions of (4-1b) without using pseudo-transient or transient methods. I call the process of solving the governing nonlinear partial differential equation by a combination of analytical and numerical techniques ASIGNing (using an Analytical Solution as Initial Guess to a Numerical solver). Figure 7.1 gives a schematic overview of the ASIGNing process.

The versatility of the approach is demonstrated for two different solutions of (4-1b) and (4-8): the case of *lognormally* distributed α (logα-case), and the case equivalent to Yeh et al. (1985a,b), where α is *normally* distributed (α-case). The former is given in (4-26). The latter is derived here: With $\alpha = A + a'$, the unsaturated hydraulic conductivity is given by:

$$\begin{aligned} \ln K(h) &= \ln K_s + \alpha h \\ &= F + f' + (A + a')(H + h') \end{aligned} \qquad \textbf{(7-2)}$$

and the governing first order perturbation equation under mean unit gradient conditions is (compare to (4-20)):

$$\frac{\partial^2 h'}{\partial x_i^2} + A\frac{\partial h'}{\partial x_1} + H\frac{\partial \alpha'}{\partial x_1} + \frac{\partial f'}{\partial x_1} = 0 \qquad i=1,2 \qquad \textbf{(7-3)}$$

The corresponding spectral solution for the head perturbation is derived equivalently to (4-26):

$$dZ_{h'} = \frac{ik_1 (dZ_{f'} + HdZ_{\alpha'})}{(k_1^2 + k_2^2 - iAk_1)} \qquad (7\text{-}4)$$

The perturbation of the normally distributed α is denoted by a' and the perturbation of the lognormal α by γ' to distinguish between the two cases.

7.3 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 a principal parameter set is chosen that allowed variations in the moments of $\log K_s$, α, and $\log\alpha$ over several orders of magnitude. The values of both the deterministic and the stochastic parameters are summarized in Table 7.1. The 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 field variables (RFVs) f', a', and γ':

$$\mathrm{Cov}(\mathbf{b}) = \sigma^2 \exp\left(\frac{-|\mathbf{b}|}{\lambda}\right) \qquad (7\text{-}5)$$

where σ^2 is the variance of the RFV, **b** is the two-dimensional vector of the separation distance, and λ = 50 cm is the isotropic correlation length.

The mean of α, (arithmetic mean A for normal α, geometric mean Γ for lognormally distributed α), determines the degree of nonlinearity in (4-1b). 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)). With α-case(1) the effect of different boundary conditions is investigated. The α-case(2) and the $\log\alpha$ case are used to demonstrate the efficiency and flexibility of the method with respect to various possible

applications.

Alternative boundary conditions are:

(a) of the Dirichlet type (prescribed head) on all boundaries;

(b) of the Dirichlet type at the top and bottom of the domain, but with zero-flux on the vertical boundaries;

(c) of the Dirichlet type at the bottom boundary, zero-flux at the vertical boundaries, and a prescribed flux of q = 7.4 cm/h at the top boundary (then H ≈ -150 cm);

(d) unit-gradient conditions at the bottom boundary, zero-flux at the vertical boundaries and prescribed flux q = 7.4 cm/h at the top boundary;

(e) water-table boundary at the bottom (uniform Dirichlet, $h_{BC} = 0$), all other boundaries are Dirichlet boundaries;

(f) water-table boundary at the bottom (uniform Dirichlet, $h_{BC} = 0$), zero-flux at the vertical boundaries, and Dirichlet boundary at the top;

(g) The logα-case is tested with boundary condition (a) and parameters similar to the α-case(1) (see Table 7.1).

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 in all example problems. All of the above boundary value cases are run at variances $\sigma^2_f = 0.1$, 1.5, and 6. Some cases are also repeated at $\sigma^2_f = 0.01$, 0.5, 1.0, and 3.0. The geometric mean of K_s is 33.1 cm/h in α-case(1) and 4.5 cm/h in α-case(2). a' and γ' are assumed to be correlated to logK_s with proportionality constants ζ = 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 unsaturated conditions are the focus of this work. The α-case(1) is also implemented with $\sigma^2_f = 1.5$ 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/stochastic parameters and the constitutive equations for K(h) and θ(h) are identical for the initial 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 (7-4) or (4-26), respectively, are used as random field input to the steady-state and transient numerical solutions (Figure 7.1).

7.4 Results and Discussion

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

It is generally known that the first-order perturbation equations (4-20) and (7-3) are a valid approximation to the nonlinear Richards equation (4-1b) for variances of $f' << 1.0$ (Yeh et al. 1985a). Hence, for problems involving only small perturbations, the quasi-analytical spectral solution technique itself is expected to be satisfactory. Figure 7.2 shows that the head field from the quasi-analytical spectral solution to (7-4) is indeed in very good agreement with the ASIGNed solution to (4-1b) at $\sigma^2_{f'} = 0.1$. At higher variances, the approximate solution deviates significantly from the "true" (numerical) solution of 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 (7-4) have artificial sources and sinks for $\sigma^2_{f'} > 0.25$. 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 (7-3) 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 (7-4), even at large variances (Figure 7.3).

This may explain, why the quasi-analytical solution provides an initial guess that allows a direct numerical steady-state solution of (4-1b) much beyond the usual limits of the first order perturbation approach.

With regard to solution uniqueness, all ASIGNed solutions are in excellent agreement with the those obtained by the time-marching approach. As an example, Figure 7.4 compares the ASIGNed with the late transient solution for α-case(1) under boundary conditions (c) at σ^2_f = 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.

7.4.2 Efficiency of the ASIGNed Solutions

The experiments show that the quasi-analytical spectral solution method to obtain (4-26) and (7-4) is an extremely CPU-efficient algorithm to obtain approximate solutions to (4-1b) (Figure 7.5). Due to its spectral nature the number of computational steps is finite and independent of σ^2_f. The savings in CPU-time over the transient time-marching numerical solution of (4-1a) is on the order of three magnitudes and more: The quasi-analytical solution of (7-3) on a discretized grid of 64*64 points takes less than 1 second 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 σ^2_f= 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 (4-1) and the main purpose 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 to 30 at any input variance (Figure 7.5). The computation time of the initial guess (1.5 sec of which almost 1 second is input/output) is

almost negligible compared to the ASIGNed numerical solution time.

While the first example in Figure 7.5 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 questionable, 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 a quasi-infinite domain. In practice, the use of random head boundaries provided by (7-4) or (4-26) is much more realistic than uniform head boundaries. The random type head boundaries are consistent in first order with the random input parameter fields $\log K_s$ and α, 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 (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 7.5 vs. 7.6).

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. But throughout the range of variability ASIGNing remains a much more efficient technique (Figure 7.6). 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 7.7). The head-field in this case is not only heterogeneous, but also deviates from the uniform mean-head assumption implicit in the initial solution (7-4). 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 7.8 shows that the efficiency of the proposed method decreases only slightly as the size of the domain increases from 1,000 to over 65,000 elements. For 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 logα-case. Table 7.2 provides some example CPU-times for both the logα-case and for the α-case(2) with much smaller mean α. The efficiency of the method is comparable to the cases shown in Figure 7.5.

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 $\text{Max}|h_{t+1} - h_t| < \delta$), since transient solutions may change very little per 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 require significantly more CPU-time than indicated in Figures 7.5 to 7.8 and in Table 7.2, since the number of time-steps required to approach steady-state are generally not a priori known.

7.4.3 Limitations of ASIGNing

The above examples have shown that ASIGNed solutions can be obtained over a wide range of variances. But it must be emphasized that the success of the method is not unlimited due to the first order character of the analytical solution. As indicated before, terms of second and higher order that were neglected in deriving the perturbation equation (7-3) and (4-20) become significant at higher variances of f' and/or a'. Hence the (initial guess) solutions (7-4) and (4-26) deviate more strongly from the steady-state solution to (4-1b) as the perturbations increase (compare Figures 7.2 and 7.3). Once the difference between the two solutions is larger than the convergence radius of the Newton-Raphson method, a direct steady-state solution is impossible to obtain even with the quasi-analytical initial guess. The experiences with the above examples have shown that ASIGNing is successful up to variances of 5 in the (natural) logarithm of the unsaturated hydraulic conductivity, $\sigma^2_{y'}$ 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 $\log\alpha$, 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 $\log\alpha$-case described above is repeated with independent parameters f' and γ'. The variances of the independent γ' in these cases are 1/100 of the variance $\sigma^2_{f'}$ specified, just as in the first $\log\alpha$ case with dependent random fields. The CPU times required for the two cases with low $\sigma^2_{f'}$ 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 $\log\alpha$ case, convergence is obtained with $\sigma^2_{f'} \leq 4.5$, which results in an unsaturated logK variance $\sigma^2_{y'} \leq 5$.

To separate the effects of f' and γ' at a given geometric mean $\alpha_g = 0.01$ [cm^{-1}], the largest $\sigma^2_{\gamma'}$ for which convergence is achieved is determined at each of three different $\sigma^2_{f'}$. At $\sigma^2_{f'} = 0.1$ and 1.5 solutions are obtained if $\sigma^2_{\gamma'} \leq 0.5$, although the range in head variance in the two cases 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 $\sigma^2_{f'} = 4.7$, the maximum usable $\sigma^2_{\gamma'}$ reduces to $2*10^{-5}$. Increasing the geometric mean of α from 0.01 to 0.1 [cm^{-1}], which is typical of a coarse sand, shows that convergence in ASIGNing is limited to slightly smaller variances of γ'. 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 $\sigma^2_{y'} = 3.0$, 4.0, and 4.2.

In the case of independent, normally distributed α the first order perturbation solution is not based on an approximation similar to (4-13). Here, ASIGNing is also successful for a large range of $A = <\alpha>$ 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 ($\sigma^2_{logK'} = 2.0$, $\sigma^2_{h'} = 235$ cm^2), and at $A = 0.5$ [cm^{-1}] it is 0.007 ($\sigma^2_{logK'} = 0.77$, $\sigma^2_{h'} = 9$ cm^2). At smaller variances of a' and $A = 0.1$ [cm^{-1}] ASIGNed solutions are generally possible if $\sigma^2_{y'} \leq 4.3$. These limits are obtained for the particular seed used to generate the random numbers α_j and β_j in (3-3). 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 (4-1). For the mean of $\alpha \leq 0.01$ or the mean of $\log\alpha \leq -4.6$, cases resulting in $\sigma^2_{y'} \leq 4$ (or even 5) are solvable with ASIGNing as long as e.g., in the $\log\alpha$ case the variance of $\gamma' \leq 0.5$. At $\alpha_g = 0.1$ and for a given $\sigma^2_{f'}$ ASIGNing is successful for any $\sigma^2_{\gamma'}$ such that $\sigma^2_{y'}$ 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 $\sigma^2_{f'}$ (if $\sigma^2_{y'}$ does not exceed 3 to 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.

7.4.4 Extensions of ASIGNing

It has already been emphasized that the boundary value problem for the initial guess, which is given by the analytical solutions (7-4) or (4-26), is different from the boundary value problems stated above for the numerical solver of (4-1b). For all the above boundary value problems the analytical solution provides an initial guess based on the assumption of an unbounded domain, while the numerical solutions are 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 analytical solutions may successfully be used as initial guess such that the steady-state finite element simulation of (4-1b) converges directly.

Theoretically, it is possible to generate quasi-analytical solutions not only with different boundary conditions than the numerical solutions, but also with a different input set $\{ F^*, \sigma^{2*}_{f'}, A^* , \sigma^{2*}_{a'}, H^* \}$ to better approximate the solution of (4-1b) 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 not only when different mean values are specified but also for different variances, if the same seed is used for the spectral random field generator: Recall from (2-49) that $dZ_p(\mathbf{k})$, p = f', a' are independent random numbers with a variance equal to the spectral density $S_{pp}(\mathbf{k})d\mathbf{k}$. Since the spectral density function $S_{pp}(\mathbf{k})$ is the Fourier transform $\mathcal{F}$ of the covariance function (7-5), 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:

$$S_{pp}(\mathbf{k}) = \sigma^2_p \, \mathcal{F}\,(Cor_{pp}(\mathbf{b}) \qquad \textbf{(7-6)}$$

where $Cor_{pp}(\mathbf{b}) = Cov_{pp}(\mathbf{b})/\sigma^2_p$ 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^2_p. They merely differ in the

amount of excitation in their perturbed structure as shown by the quasi-analytical solutions in Figures 7.2 and 7.3. The same is not true for the head solution to (4-1b) due to its nonlinear character. Yet the structures are similar as shown by the ASIGNed head solution in Figure 7.2 produced from random fields of correlated f' and a' with $\sigma^2_{f'} = 0.1$ and the ASIGNed head solution shown in Figure 7.3 which is based on random fields with $\sigma^2_{f'} = 6.0$.

It is therefore conceivable to generate the initial guess solution with a meaningful, but arbitrary set of parameters { F*, $\sigma^{2*}_{f'}$, A* , $\sigma^{2*}_{a'}$, H* }, to produce a certain structure in the initial head h', which is closer to the solution of (4-1b) subject to { F, $\sigma^2_{f'}$, A, $\sigma^2_{a'}$, H } than an initial head that is also based on { F, $\sigma^2_{f'}$, A, $\sigma^2_{a'}$, H }. The practical procedure is then as follows: After obtaining the initial head h' with an arbitrary set { F*, $\sigma^{2*}_{f'}$, A* , $\sigma^{2*}_{a'}$, H* }, one regenerates f' and a' with the same seed, but the input set { F, $\sigma^2_{f'}$, A, $\sigma^2_{a'}$, H }, and then proceeds 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 (f) 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 principal, ASIGNing can also be applied for cases where a solution to (4-1b) is sought with an unsaturated conductivity function K(h) different from (4-8). In this case the moments of the parameters K_s and α in (4-8) have to be determined such that the head field from (7-4) is similar to that solving (4-1b) with the desired K(h) function. A prominent example is the use of Van Genuchten's constitutive relationships for K(h) and θ(h) (Van Genuchten, 1980) in the numerical solution of (4-1b). While Gardner's equation for K(h) (4-8) is necessary for the derivation of (7-4), 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 (4-1b) may be possible by defining equivalent parameters

f' and a' for (4-8) analytically (Russo et al., 1991). This is cumbersome, however, since an equivalent f' and a' need to be determined for each random replicate of VanGenuchten parameters. Alternatively, the equivalent moments { F^*, $\sigma^{2*}_{f'}$, A^* , $\sigma^{2*}_{a'}$ } of the K(h) parameters in (4-8) can be graphically matched by trial and error with those desired for the VanGenuchten K(h): The parameter set { F^*, $\sigma^{2*}_{f'}$, A^* , $\sigma^{2*}_{a'}$ } 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 (e.g. Ababou, 1988, p.652). 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.

7.5 Conclusions

In many instances and particularly in the case of heterogeneous, steady, non-linear 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 non-uniform. For problems involving heterogeneous parameter-fields e.g., flow through variably permeable porous media, such an initial guess is commonly 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.

A quasi-analytical spectral solution technique was developed, which is a first-order linearized perturbation approximation to the governing non-linear 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 (4-1b) (ASIGNing: Analytical Solution as Initial Guess to Numerical solver). ASIGNing renders up to two orders of magnitude of CPU-time savings. To my knowledge this is the first time stochastic analytical solutions have been

combined with their respective numerical solutions. It was shown that the method 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, if the parameters for the initial guess solutions are determined separately. In this chapter examples are shown, where the set of parameters for both the initial guess and the numerical solution are identical (with the exception of the mean head). ASIGNing works for correlated and uncorrelated f' and a' fields alike, and can be adopted to solve problems involving normal or lognormally distributed α. The success of this particular combination of a quasi-analytical with a numerical method is very encouraging since the nature of the 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. Alternatively, partial boundary conditions can be introduced through conditional simulation techniques, a possibility that is investigated in chapter 10. 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. Subsequent chapters will explore several different such applications of ASIGNing.

Table 7.1: Parameters for the numerical experiments

	α-case(1) and logα-case	α-case(2)
mean $\log K_s$ [cm/d]	3.5	1.5
variance σ^2_f	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 logα: Γ [1/cm]	-4.6	-
$\zeta_{\gamma'f}=\sigma_{\gamma'}/\sigma_f$	0.1	-
mean head: H [cm]	-150	-150

Table 7.2: Results of the α-case(2) and the logα-case experiments

	σ^2_f (saturated hydraulic cond.)	$\sigma^2_{[\log K]'}$ (unsatur. hydraulic cond.)	CPU-time[sec] (pseudo-transient)	CPU-time [sec] (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
logα-case	0.1	0.062	563	16.6
logα-case	1.5	0.96	743	39.4
logα-case	6.0	3.99	N/A*	63.9

* N/A: transient solution did not converge

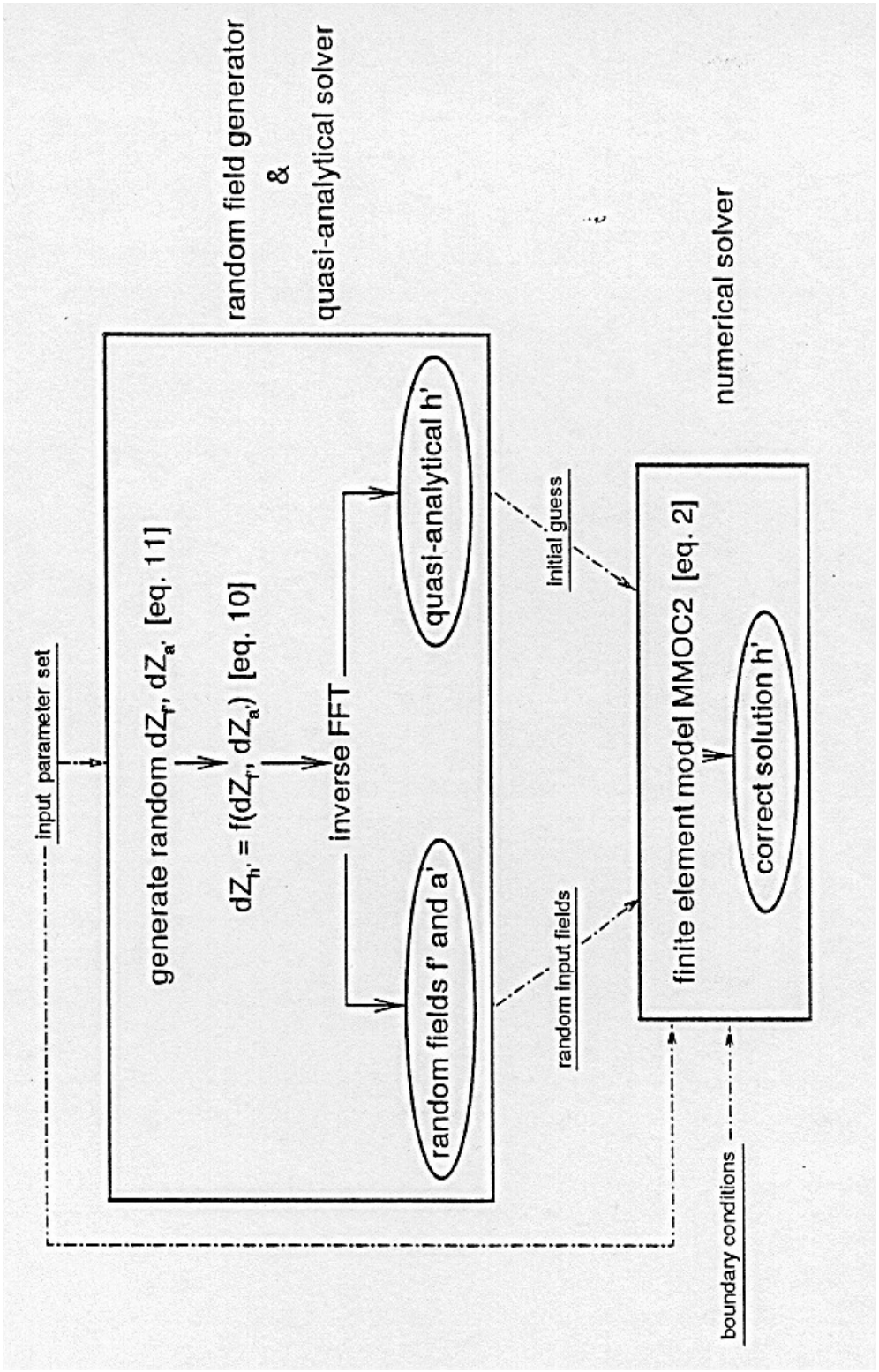
input parameter set
generate random dZ_f, dZ_a, [eq. 11]
$dZ_{h'} = f(dZ_f, dZ_{a'})$ [eq. 10]
inverse FFT
random fields f' and a'
quasi-analytical h'
random field generator
&
quasi-analytical solver
random input fields
initial guess
finite element model MMOC2 [eq. 2]
correct solution h'
numerical solver
boundary conditions

Figure 7.1:

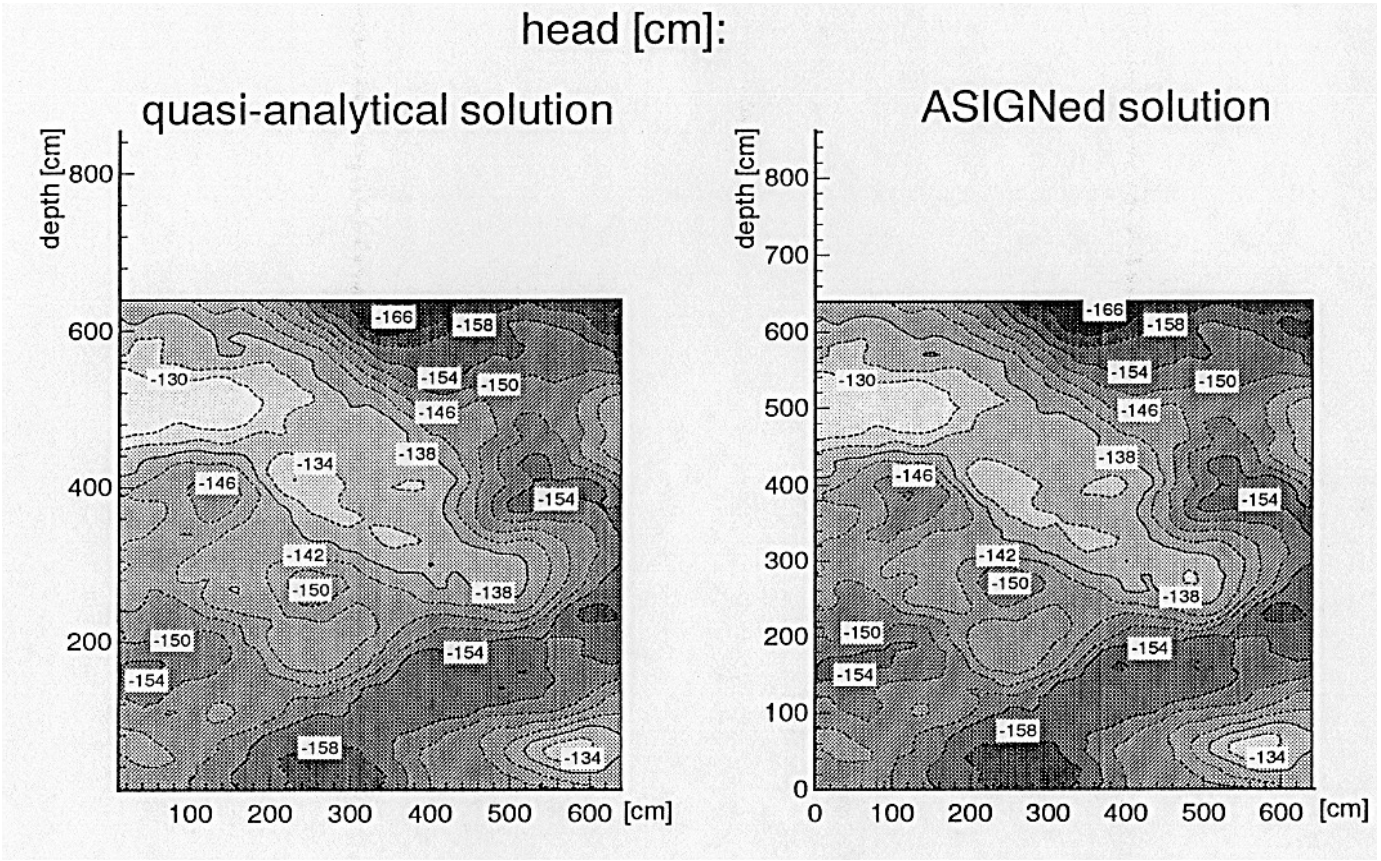

Figure 7.2:

spectral method with the ASIGNed finite element solution to Richards equation under boundary condition (a) at

$\sigma_f^2 = 0.1$. The labels indicate the head [cm] at the nearest contour line.

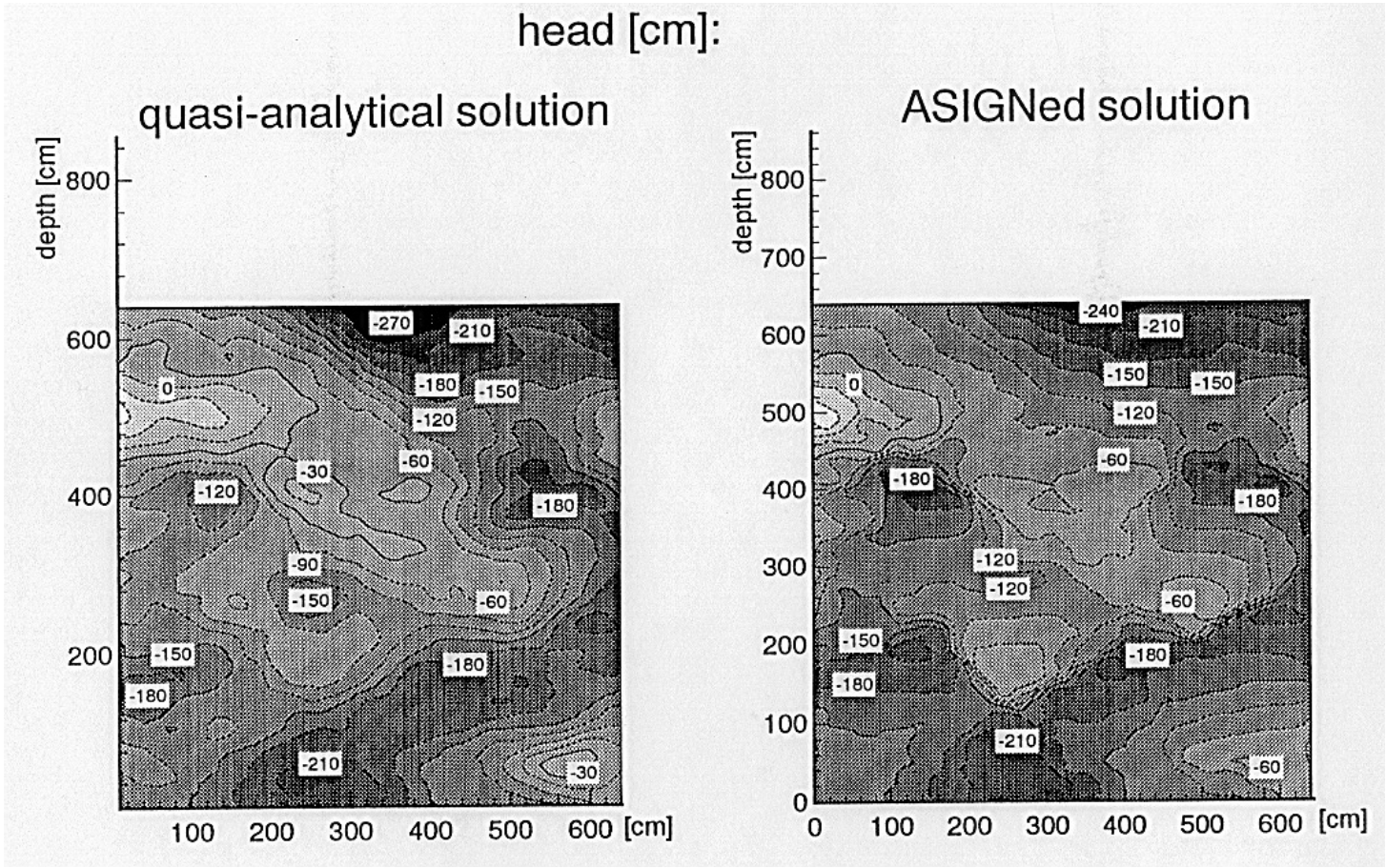

Figure 7.3:

with the ASIGNed finite element solution to Richards equation under boundary condition (a) at indicate the head [cm] at the nearest contour line.

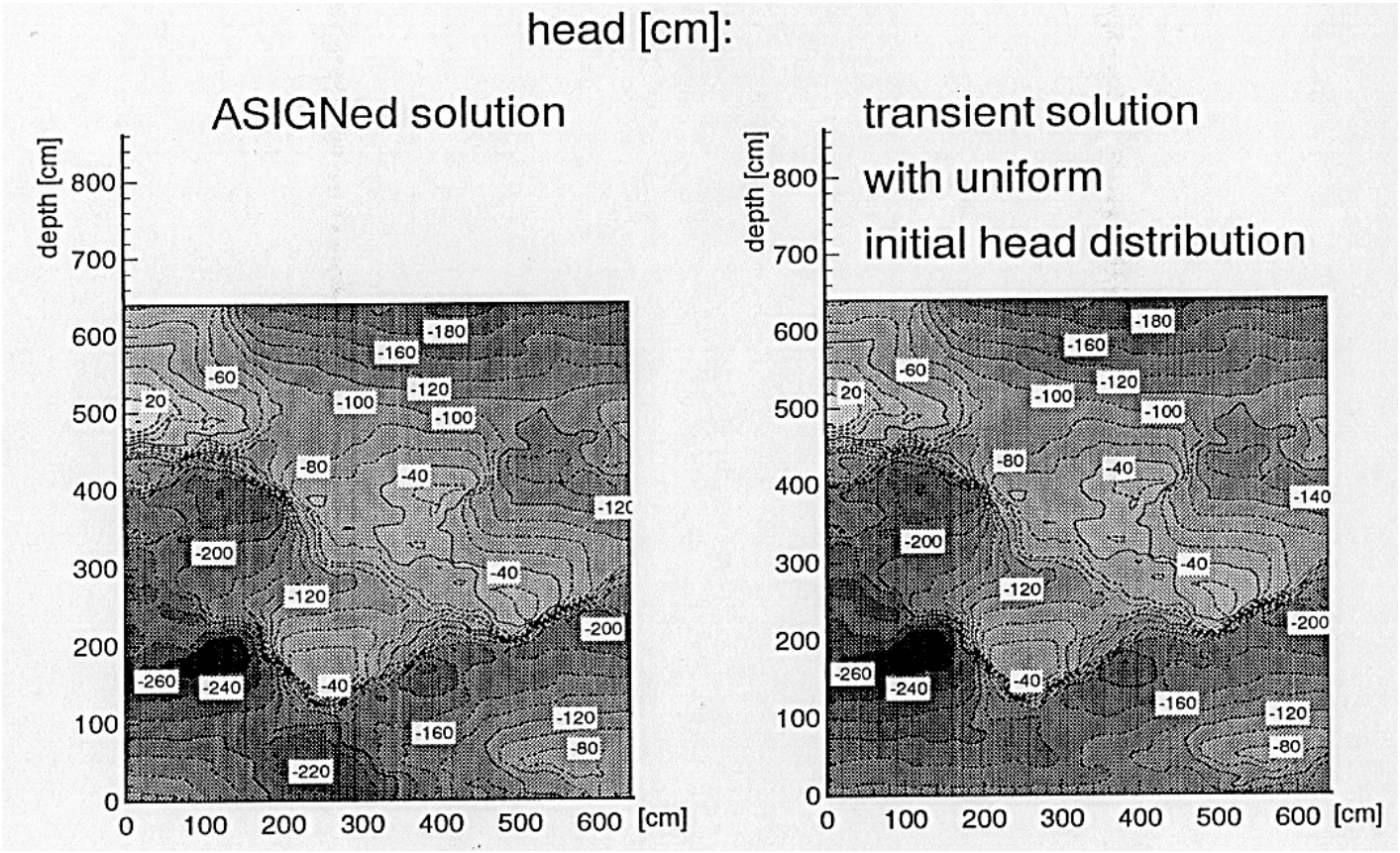

Figure 7.4:

element solution to Richards equation with that obtained by transient time-marching
indicate the head [cm] at the nearest contour line.

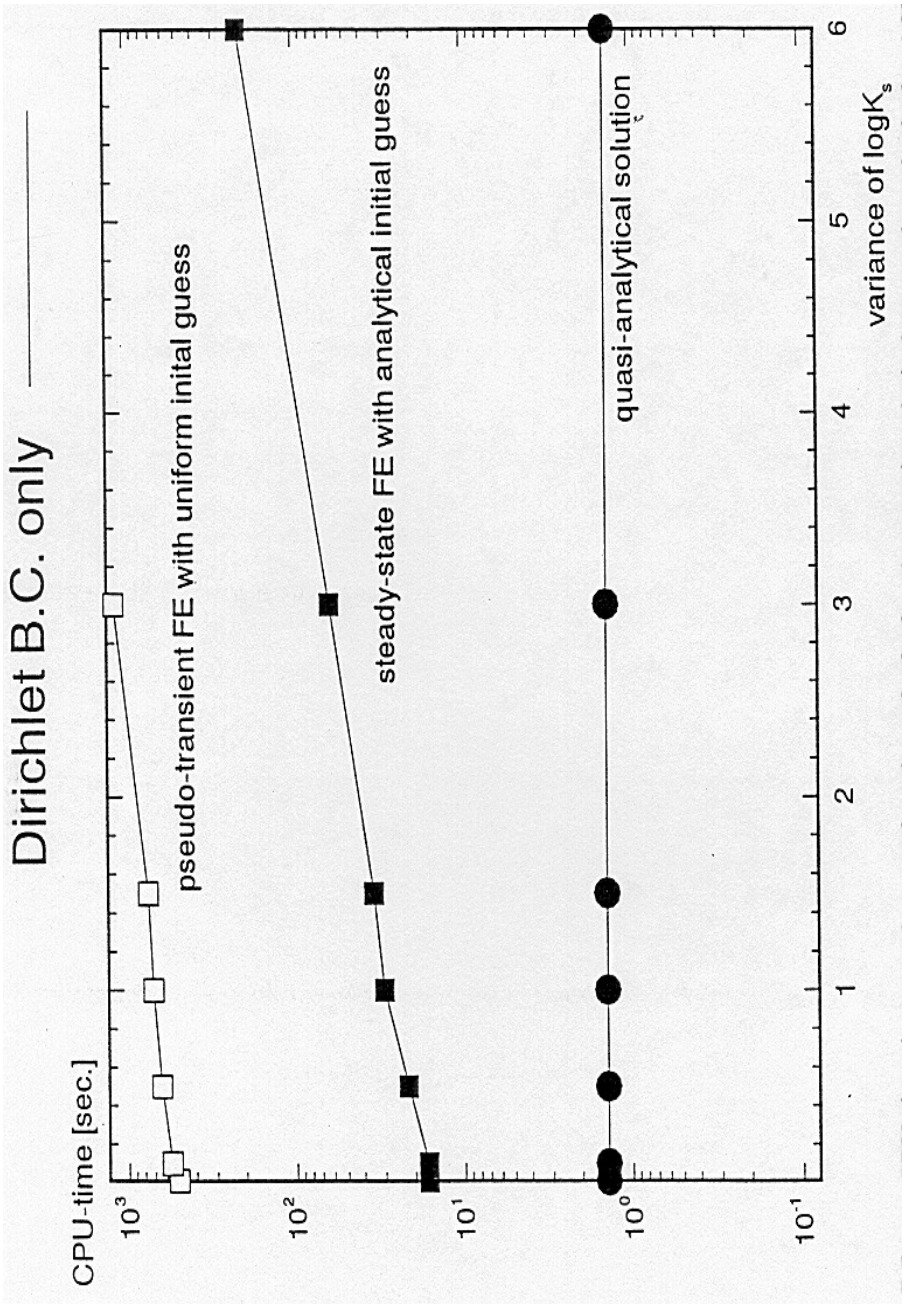

Figure 7.5: ASIGNed numerical solution (without computation of the initial guess), and the transient numerical solution with a uniform initial head distribution. The numerical cases are computed with boundary conditions (a).

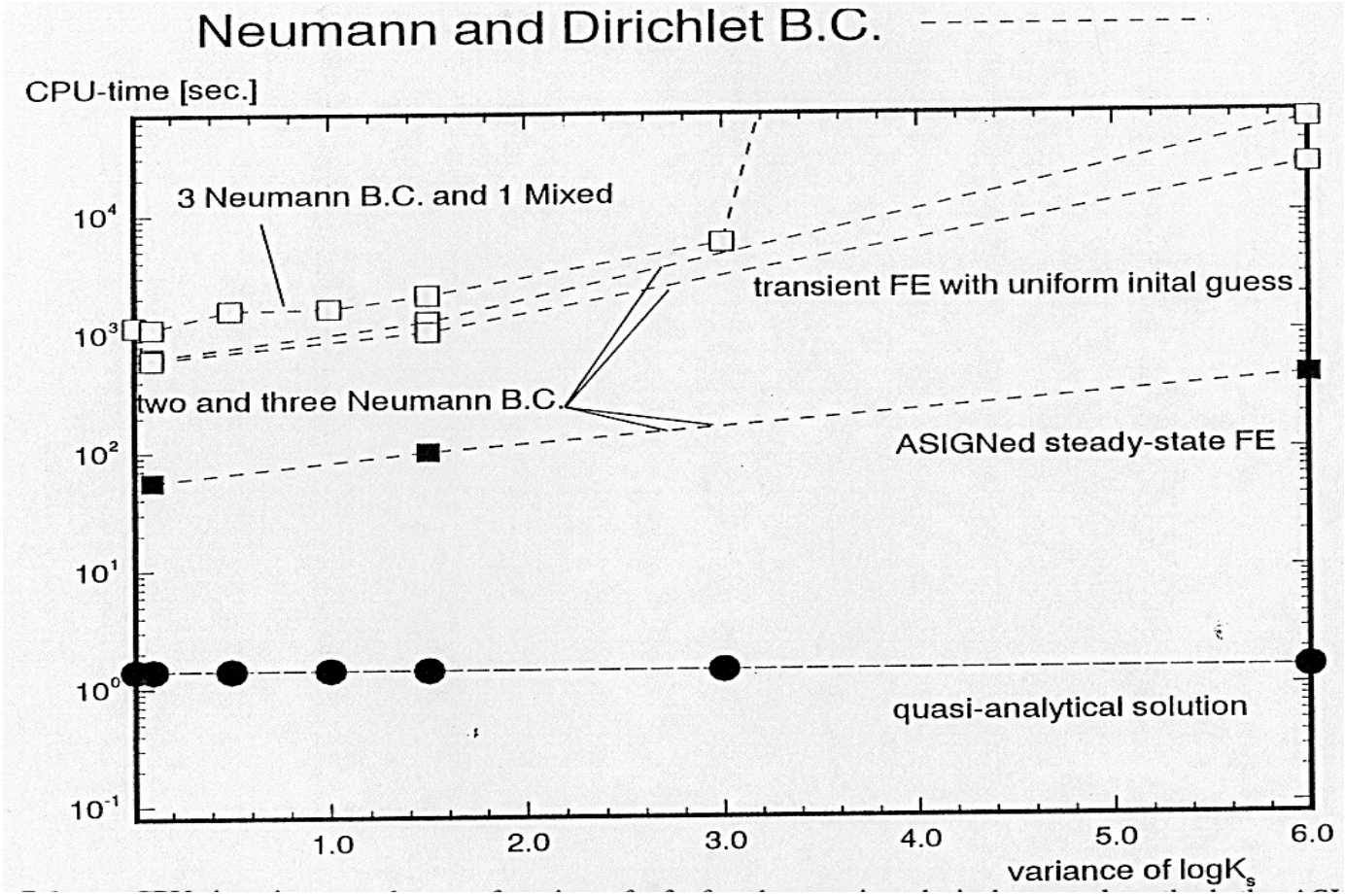

Figure 7.6:

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 (b) and (c). No convergence in the ASIGNed solution was achieved for boundary condition (d).

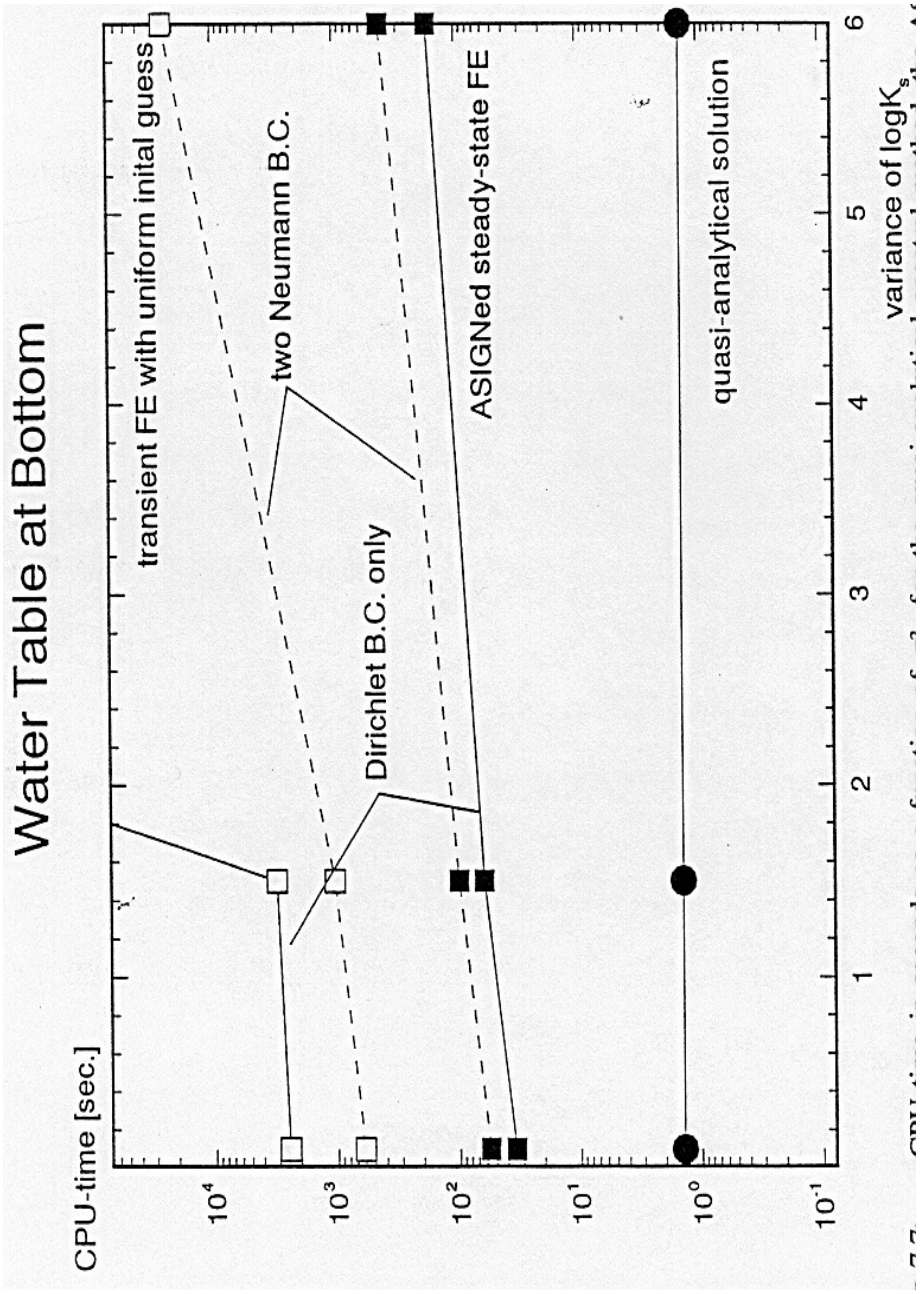

Figure 7.7: numerical solution (without computation of the initial guess), and the transient numerical solution with a uniform initial head distribution. The numerical cases are computed with boundary conditions (e) and (f).

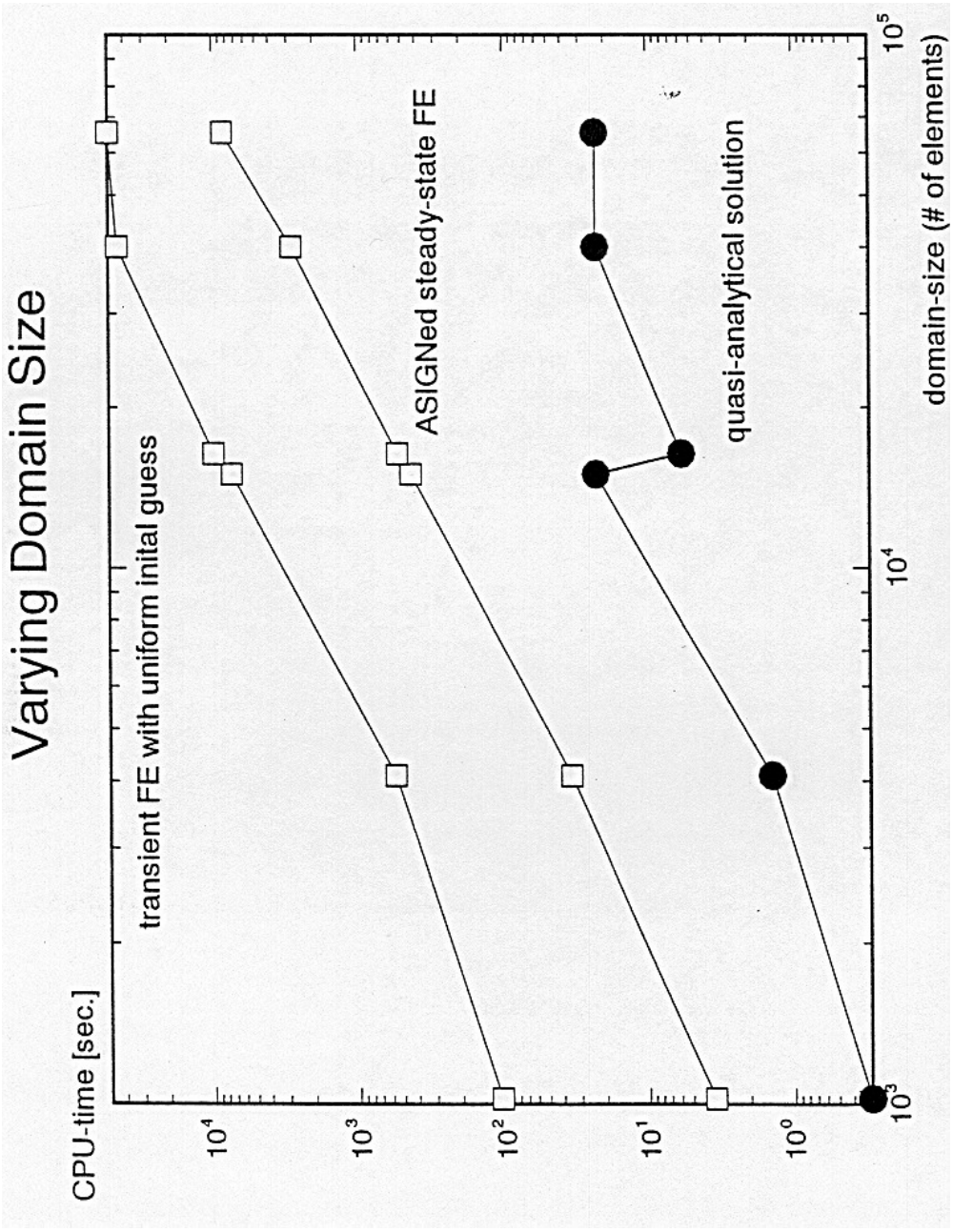

Figure 7.8: method, the ASIGNed numerical solution (without computation of the initial guess), and the transient numerical solution with a uniform initial head distribution. The numerical cases are computed with boundary conditions (a).