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A new convergence criterion for the modified Picard iteration method to solve the variably saturated flow equation

K. Huang, B.P. Mohanty, M.Th. van Genuchten*

US Salinity Laboratory, USDA, ARS, Riverside, CA 92507, USA

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Abstract

Solutions of the Richards equation for water flow in variably saturated porous media are increasingly being used in water resources evaluation and environmental management. Besides the accuracy of solution, also of concern is the required computational effort, especially when highly nonlinear soil hydraulic properties and dry initial conditions are involved. In this paper we evaluate the performance of different convergence criteria when the modified Picard iteration method is used for solving the mixed-form Richards equation. Results are compared in terms of computer processing (CPU) time and number of iterations. A new nonlinear convergence criterion derived using a Taylor series expansion of the water content was implemented in the mixed-form numerical algorithm. The computational efficiency of the new criterion was evaluated against two widely used convergence criteria for different soil types, boundary conditions, initial conditions, and layered soils. Whereas all three criteria produced nearly identical results in terms of calculated water content, pressure head, and water flux distributions, all with negligible mass balance errors, the required CPU times were significantly different. In general, the new nonlinear convergence criterion was found to be computationally much more efficient than the other two criteria. The new criterion was also more robust (i.e. the solution remained convergent) for highly nonlinear flow problems for which the other two convergence criteria failed. Results of this study indicate that the new convergence criterion, when implemented in the modified Picard solution of the mixed-form Richards equation, produces a very efficient and accurate method for simulating variably saturated water flow in soils.

1. Introduction

Numerical models are important tools in environmental studies to assess the risks of groundwater contamination from chemicals released in the unsaturated zone. The

* Corresponding author.

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extreme variability and complexity of geological materials, dry initial conditions, and varying boundary conditions can make the flow and transport problem difficult to solve within acceptable limits of accuracy and computational effort. Most of the currently available numerical methods have sacrificed either accuracy or computational efficiency. For example, infiltration into relatively coarse-textured soils is generally difficult to model because of highly nonlinear hydraulic characteristics. Dry initial conditions and highly nonlinear hydraulic properties often require the use of very fine spatial and temporal discretizations to avoid numerical instabilities. These conditions cause numerical algorithms to become CPU-intensive, especially when long-term and/or multi-dimensional problems must be simulated. Hence, efforts to achieve the best numerical algorithm should involve optimizing both the accuracy and robustness of the scheme, as well as minimizing the required computational time.

The objective of this paper is to improve the computational efficiency of the mixed-form algorithm of Celia et al. (1990) for solving variably saturated flow problems. Improvements were made by accelerating the rate of convergence through a new nonlinear convergence criterion. The proposed criterion will be evaluated by comparing its performance with two other popularly used convergence criteria.

2. Background

One-dimensional vertical flow of water in a variably saturated rigid soil under isothermal condition is generally described with the Richards equation (Richards, 1931), which may be written in terms of either the pressure head, i.e.

$$C\frac{\partial h}{\partial t} = \frac{\partial}{\partial z}\left(K\frac{\partial h}{\partial z} - K\right) - S \tag{1}$$

or the water content, i.e.

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}\left(D\frac{\partial \theta}{\partial z}\right) - \frac{\partial K}{\partial z} - S \tag{2}$$

where h is the pressure head (L), θ is the volumetric water content ($L^3\ L^{-3}$), t is time (T), z denotes the vertical distance from the soil surface downward [L], $C = \mathrm{d}\theta/\mathrm{d}h$ is the specific water content capacity (L^{-1}), K is the hydraulic conductivity ($L\ T^{-1}$), $D = K/C$ is the soil water unsaturated diffusivity ($L^2\ T^{-1}$), and S is a source/sink term (T^{-1}).

Until recently, most numerical studies have used either the h- or θ-based form of the Richards equation to describe flow in a variably saturated soil (e.g. Davis and Neuman, 1983; Huyakorn et al., 1983, 1989; Hills et al., 1989; Kool and Van Genuchten, 1991; Kirkland et al., 1992). Water-content-based schemes using Eq. (2) may be written in a mass-conservative form and hence should in most cases conserve mass within the computation domain regardless of time step and grid spacing (Hills et al., 1989). Huyakorn and Pinder (1983) showed that it is advantageous to use such schemes for initially dry homogeneous soils. A limitation of the θ-based formulation is that this form cannot be used to describe flow in the saturated zone, and flow in layered soils is also not easily simulated. Furthermore, θ-based algorithms may suffer from mass balance errors at the boundaries even when this formulation accurately conserves mass in the interior of the flow system. The h-based formulation (1) is considered to be more useful for practical problems involving flow in layered or spatially heterogenous soils, as well as for variably saturated flow problems. Unfortunately, simulation of infiltration in dry and/or high nonlinear soils using the h-based formulation often faces difficulties in conserving mass. A more detailed discussion of the relative advantages and disadvantages of h-based and θ-based forms of the Richards equation has been given by Hills et al. (1989).

Several researchers have explored alternative numerical techniques for solving the h- or θ-based forms of the Richards equation. The objectives of these studies include obtaining more stable numerical algorithms, speeding up the calculations, minimizing mass balance errors, and achieving more accurate solutions for different soil types or initial and boundary conditions. For example, Milly (1985) presented a mass-conservative solution procedure in which an effective element soil water capacity term was used. This approach, coupled mass lumping (Neuman, 1973), effectively insures global mass balance with the h-based equation. Rathfelder and Abriola (1994) developed similar mass-conservative solutions for the h-based equation by expanding and discretizing the soil water capacity. Others have used Kirchhoff type transformations (e.g. Ross and Bristow, 1990) or alternative functions (Ross, 1990; Pan and Wierenga, 1995) to facilitate less nonlinear flow descriptions. In a different approach, Gottardi and Venutelli (1992) used a moving finite-element method in which grid points move along the wetting front, thereby permitting fewer nodes without sacrificing numerical accuracy. The moving grid method, however, has several limitations when applied to layered systems or used with time-varying boundary conditions. This method was also found to be less mass-conservative than conventional fixed-grid formulations. El-Kadi and Ling (1993) proposed Peclet and Courant number criteria for spatial and temporal discretizations, to describe the accuracy and efficiency of numerical schemes solving the Richards equation. By introducing a source term, Hills et al. (1989) successfully solved the problem involving one-dimensional water flow into layered soils with the θ-based algorithm. Kirkland et al. (1992) subsequently developed a θ-based algorithm involving a transformation of variable to model variably saturated flow in two dimensions. More recently, Huang et al. (1994) proposed a method-of-characteristics based particle tracking technique to solve the h-based Richards equation for highly nonlinear infiltration problems.

Perceiving the drawbacks of existing h- and θ-based solutions of the Richards equation, many have tried to combine the advantages of the two methods. The mixed form of the Richards equation was thought to maintain the mass conservative property inherent in the θ-based equation, while providing solutions in terms of the pressure head, h. The mixed-form formulation of Richards equation is written as

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}\left(K\frac{\partial h}{\partial z}\right) - \frac{\partial K}{\partial z} - S \tag{3}$$

Brutsaert (1971) was one of the first to use the mixed-form Richards equation for solving saturated–unsaturated flow. He combined a finite difference approximation of the mixed-form equation with a Newton iteration scheme to deal with steep wetting fronts effectively. Allen and Murphy (1985, 1986) used a mixed form of the Richards equation in their collocation finite element algorithm with 'quasi-Newton' iteration. More recently, Celia et al. (1987) and Celia et al. (1990) proposed a mass-conservative numerical scheme to solve the mixed-form Richards equation (3) using 'modified Picard iteration'. Because of a perfect mass balance, the modified Picard iteration technique proved to be a major improvement over earlier Picard methods. The modified Picard iteration method also showed much promise in modeling unsaturated flow with steep wetting fronts (Celia et al., 1990; Celia and Bining, 1992). Ray and Mohanty (1992) subsequently revisited the mixed-form algorithm and showed its advantages over h-based schemes by means of several numerical experiments.

Similarly to the h- and θ-based algorithms, the modified Picard iteration scheme of Celia et al. (1990) is based on a fully implicit (backward Euler) time approximation of Eq. (3) as follows:

$$\frac{\theta^{n+1,m+1} - \theta^{n}}{\Delta t} - \frac{\partial}{\partial z}\left(K^{n+1,m}\frac{\partial h^{n+1,m+1}}{\partial z}\right) + \frac{\partial K^{n+1,m}}{\partial z} = 0 \tag{4}$$

where the superscripts n and m denote time level and iteration level, respectively, and where for simplicity the sink term, S, has been ignored. However, instead of directly solving the discretized equation, the water content at the new time step and iteration level ($\theta^{n+1,m+1}$) is replaced with a truncated Taylor series expansion with respect to h about the expansion point $h^{n+1,m}$, i.e.

$$\theta^{n+1,m+1} = \theta^{n+1,m} + \left(\frac{\mathrm{d}\theta}{\mathrm{d}h}\right)^{n+1,m}(h^{n+1,m+1} - h^{n+1,m}) + O[(\delta^{m})^{2}] \tag{5}$$

where

$$\delta^{m} = h^{n+1,m+1} - h^{n+1,m} \tag{6}$$

is the difference between the solved pressure heads at the m and $m+1$ iteration levels. Neglecting the higher-order terms in (5) and substituting this equation into (4) gives

$$C^{n+1,m}\frac{h^{n+1,m+1} - h^{n+1,m}}{\Delta t} + \frac{\theta^{n+1,m} - \theta^{n}}{\Delta t} - \frac{\partial}{\partial z}\left[K^{n+1,m}\left(\frac{\partial h^{n+1,m+1}}{\partial z} - 1\right)\right] = 0 \tag{7}$$

which can be rewritten as

$$\left(\frac{1}{\Delta t}C^{n+1,m}\right)\delta^{m} - \frac{\partial}{\partial z}\left(K^{n+1,m}\frac{\partial \delta^{m}}{\partial z}\right) = \frac{\partial}{\partial z}\left(K^{n+1,m}\frac{\partial h^{n+1,m}}{\partial z}\right) - \frac{\partial K^{n+1,m}}{\partial z} - \frac{\theta^{n+1,m} - \theta^{n}}{\Delta t} \tag{8}$$

Eq. (8) defines the modified Picard approximation of Celia et al. (1990) as applied to the mixed-form Richards equation. It should be noted that δ^m in (8) is now the unknown dependent variable rather than the pressure head $h^{n+1,m+1}$. Once δ^m is solved by any standard technique such as finite elements or finite differences, the desired solution for the pressure head $h^{n+1,m+1}$ can be obtained from (6). The last term on the right-hand side of Eq. (8) corresponds to the time derivative and is a key term to obtaining perfect mass balance.

Celia et al. (1990) claimed that the mass-conservative property of Eq. (8) holds for all types of boundary conditions and all numerical approximations that maintain spatial symmetry. However, they also pointed out that as the left-hand side of (8) for the modified Picard scheme is identical to that of the original Picard formulation involving the h-based Richards equation, the computational effort for both forms should be identical, and hence there should be no computational advantage of using the mixed-form algorithm as opposed to the h-based formulation. Our study is designed to implement a new nonlinear convergence criterion in conjunction with the above mixed-form algorithm of Celia et al. (1990) to improve further the computational efficiency as compared with standard convergence criteria used in most current numerical studies.

3. Proposed convergence criterion

In numerical simulations using the h-based form of the Richards equation, the value of the pressure head at a new time level is usually guessed at first, and subsequently improved iteratively. The iterative process continues until the difference between the calculated values of the pressure head between two successive iteration levels becomes less than a preset tolerance δ_a, i.e. until the following inequality is satisfied at all nodes:

$$|\delta^m| = |h^{n+1,m+1} - h^{n+1,m}| \leqslant \delta_a \tag{9}$$

This convergence criterion has been relatively standard in numerical studies, with the value of δ_a varying widely. For example, while simulating three-dimensional unsaturated flow in a soil slab using finite elements, Huyakorn and Wadsworth (1985) adopted $\delta_a = 0.01$ cm and 0.001 cm as the convergence tolerances for Picard iteration and slice successive over-relaxation (SSOR) matrix subiteration, respectively, but used $\delta_a = 1$ cm for drainage simulations. The soils in their examples were initially relatively wet. Although it is generally true that more accurate solution can be obtained with smaller values of the convergence tolerance, δ_a, the computational time required to reach a convergent solution using small values of δ_a can become excessive, especially for very nonlinear infiltration problems.

In efforts to reduce the computational requirements associated with a small tolerance, δ_a, in (9), several workers (e.g. Cooley, 1983; Kaluarachchi and Parker, 1989; Kool and Van Genuchten, 1991) suggested the use of an empirical convergence criterion which involves both an absolute error (δ_a) and a relative error (δ_r) as follows:

$$|\delta^m| = |h^{n+1,m+1} - h^{n+1,m}| \leqslant \delta_r |h^{n+1,m+1}| + \delta_a \quad (10)$$

This convergence criterion is referred to hereafter as the mixed convergence criterion. Values adopted for the relative tolerance, δ_r, have generally ranged from 0.001 to 0.01 depending upon the desired accuracy. Eq. (10) shows that the relative part $\delta_r|h^{n+1,m+1}|$ can become large in comparison with the absolute part δ_a when the absolute value of the pressure head $h^{n+1,m+1}$ is high. Although this suggests that convergent solutions are now more easily obtained as compared with the standard convergence criterion (9), the converged solutions using (10) may be substantially different from those predicted with the standard criterion. Because of a less strict convergence criterion, errors in the calculated pressure head using (10) may become unacceptable for certain applications where accurate estimates of the pressure head or fluid flux are required, such as near sharp moisture fronts. For such applications, the mixed criterion will serve to reduce the number of iterations, in particular when the pressure head changes significantly but the water content only little.

Celia et al. (1990), and subsequently others, invoked the standard convergence criterion (9) to judge the convergence status of their mixed-form algorithm. As discussed above, this standard criterion is valid for h-based algorithms, but may be used also for the mixed-form algorithm of Celia et al. (1990), as this scheme actually solves for the pressure head $h^{n+1,m+1}$, as for the h-based formulation. However, a different formulation arises if one considers the Taylor series expansion (5) of $\theta^{n+1,m+1}$ as the core of the modified Picard iteration method. This expansion suggests that the entire storage term ($C^{n+1,m}\delta^m$) of the right-hand side of (5), rather than only the absolute error δ^m, should be included in the convergence criterion. In other words, instead of (9), we propose to use the following criterion for the mixed-form algorithm

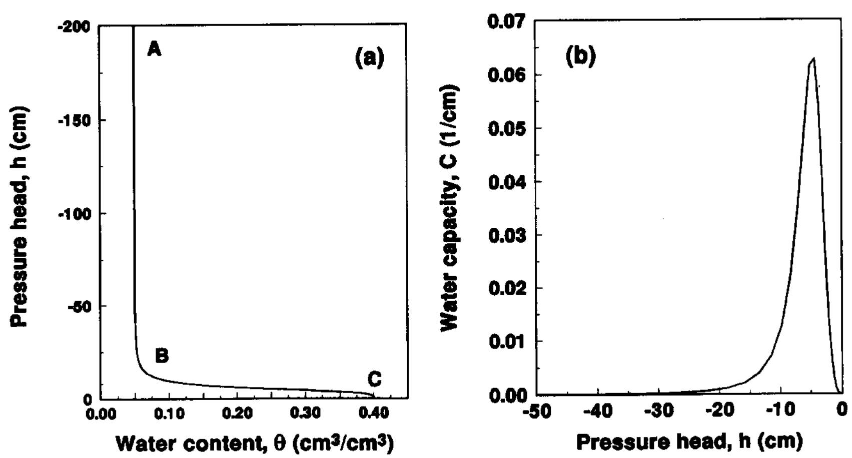

Fig. 1. Typical soil water retention and capacity curves for a coarse-textured soil.

of Celia et al. (1990):

$$C^{n+1,m}|\delta^m| = |\theta^{n+1,m+1} - \theta^{n+1,m}| \leqslant \delta_\theta \tag{11}$$

This new criterion seems more appropriate than both (9) and (10) from a mathematical point of view, and because of physical considerations. Figs. 1(a) and 1(b) present typical soil water retention and water capacity curves, respectively, for a relatively coarse-textured soil. Considering the AB part of the retention curve at the lower water contents, one may expect that if the pressure head changes significantly within this range, many iterations will be required to obtain a convergent solution with standard criterion (9) using a value of, for example, 1 cm for δ_a. On the other hand, θ within this range changes only minimally, resulting in a very small or nearly zero value of the soil water content capacity, C (Fig. 1(b)). Thus, even though $|\delta^m|$ is relatively large, the product ($C^{n+1,m}|\delta^m|$) is still small to the point of being negligible in Taylor series expansion (5). In other words, the number of iterations, and hence the computational effort, should be reduced by allowing a relatively large absolute error $|\delta^m|$ for regions where the soil is dry but changes in the water content are still small. A similar reasoning applies to the θ range very close to saturation, although the advantages of the new criterion may not be immediately obvious here because of a much smaller range in pressure heads within this region. More interesting results can be found within the θ range BC where the water content changes dramatically with small changes in the pressure head. The water capacity term generally reaches a maximum within this region, usually of the order of $10^{-4} \sim 10^{-1}$ cm^{-1} depending upon soil type. Numerical results for the standard criterion become now very sensitive to the value of the tolerance, δ_a. For example, if $\delta_a = 1$ cm is used, convergence will be relatively rapid, but a large error in θ is now likely. Hence, a much smaller δ_a should be used in the BC region to avoid large errors in θ. By contrast, the proposed nonlinear criterion will avoid some of these difficulties by specifying a tolerance on θ, e.g. $\delta_\theta = 0.0001$,

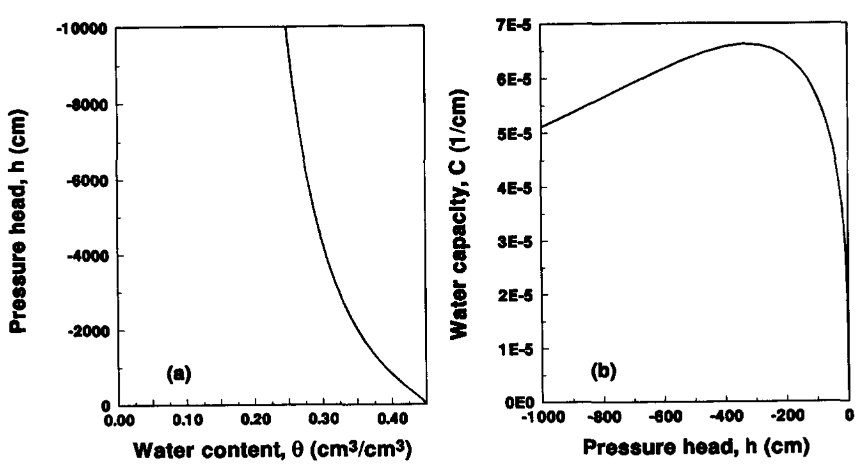

Fig. 2. Typical soil water retention and capacity curves for a fine-textured soil.

thereby automatically requiring $|\delta^m|$ to reduce to an appropriate value when the water capacity C becomes relatively large. As opposed to the curves for the coarse-textured soil in Fig. 1, the soil water retention and capacity curves for a typical fine-textured soil (Fig. 2) are less nonlinear, such that the advantages of the proposed criterion may not be as significant as for a coarse-textured soil.

We will now evaluate for several example problems the performance of the new criterion (11) in terms of solution accuracy and, particularly, computational efficiency.

4. Numerical experiments

Several hypothetical infiltration problems were simulated for the purpose of evaluating the relative performance of the different convergence criteria. Numerical experiments were conducted for soils with different hydraulic characteristics. We also studied the effects of different initial and boundary conditions, as well as soil layering, on the results. For simplicity, we solved (7) instead of (8) to obtain directly solutions for the pressure head using the mass-lumped Galerkin finite element method. The soil water retention and hydraulic conductivity were described by Van Genuchten (1980) as

$$S_e = \frac{\theta - \theta_r}{\theta_s - \theta_r} = \frac{1}{[1 + (\alpha|h|)^n]^{1-1/n}} \tag{12}$$

$$K = K_s S_e^{1/2}[1 - (1 - S_e^{n/(n-1)})^{1-1/n}]^2 \tag{13}$$

where S_e is effective saturation; θ_r and θ_s are the residual and saturated water contents ($L^3\ L^{-3}$), respectively; K_s is the saturated hydraulic conductivity ($L\ T^{-1}$); $\alpha(L^{-1})$ and n are shape parameters. Except where mentioned otherwise, we fixed the hydraulic parameters for all numerical experiments at $K_s = 100$ cm day^{-1}, $\theta_s = 0.45$, and $\theta_r = 0.05$. In each case we used a relative tolerance $\delta_r = 0.001$, an absolute tolerance $\delta_a = 1$ cm, and $\delta_\theta = 0.0001$.

Two types of boundary conditions were used at the soil surface ($z = 0$): (1) a flux boundary condition assuming a constant infiltration rate of 50 cm day^{-1}; (2) a ponding boundary condition with zero head. All examples were run with a free-drainage or unit-gradient condition (McCord, 1991) at the bottom boundary. For simplicity, each simulation assumed a uniform initial pressure head in the soil profile. Numerical results were obtained by implementing the different convergence criteria into the computer code HYDRUS (Version 5.0) (Vogel et al., 1995), which is a revised and updated version of the original HYDRUS code developed by Kool and Van Genuchten (1991). The updated code simulates one-dimensional water flow, solute transport, and heat movement in variably saturated porous media using a linear finite element algorithm. The flow problem was solved using the modified Picard iteration method applied to the mixed-form Richards equation. All simulations invoked a solution domain of 200 cm, constant spatial increments (Δz) of 2 cm, and a maximum permitted number of iterations of 20. Although the initial, minimum and maximum values of the time steps were the same for all numerical experiments, the actual time step, Δt, was automatically updated according to the convergence history during a simulation run. Simulations were run on a 486/33 MHz 16 bit personal computer. Real-run (CPU) times reported in this paper include times for reading and writing files (generally only a very small fraction of the total CPU time).

The three convergence criteria for the mixed-form algorithm were evaluated in terms of solution quality (including mass balance error (MBR) and solution accuracy) and computational efficiency (CPU time and total number of iterations during the simulations). For comparison purposes, we considered the numerical solution obtained using the absolute convergence criterion with δ_a set at 1 cm to be the 'exact solution'. This solution was in most or all cases indistinguishable from results obtained with a tolerance δ_a of 0.01 cm. The accuracy and computational efficiency of the solutions using the mixed and proposed criteria were then evaluated by comparisons with the exact results. Based on the flow continuity equation, the mass balance error (MBR) was defined as the difference of the net amount of water added to the system and the change in the amount of water stored in the system after a given elapsed time.

5. Results and discussion

Figs. 3(a), 3(b), and 3(c) show simulated water content (θ), pressure head (h), and Darcian fluid flux (q) distributions, respectively, using three convergence criteria, i.e. the proposed nonlinear criterion δ_θ given by Eq. (11), the mixed criterion $(\delta_r|h| + \delta_a)$ given by (10), and the standard criterion δ_a given by (9). The distributions are for infiltration at a constant flux of 50 cm day^{-1} in a coarse-textured soil with hydraulic parameters $\theta_r = 0.05$, $\theta_s = 0.45$, $K_s = 100$ cm day^{-1}, $n = 5.0$ and $\alpha = 0.2$ (Exp. 4, Table 1). Essentially the same numerical results were obtained for all three convergence criteria. The closeness of results for different convergence criteria was found to be a general rule rather than an exception. Moreover, when the mixed-form algorithm of Celia et al. (1990) was used, the three criteria in all cases produced perfect mass balances ($|\mathrm{MBR}| < 10^{-14}$). Although a zero mass balance error does not necessarily imply a correct numerical solution, mass conservation is at a minimum a requisite for an accurate numerical solution. As the solutions in all cases were very close and consistent, and had correct mass balances, we shall further compare the performance of the three convergence criteria only in terms of the required CPU times and total number of iterations for the simulations. CPU times for the example of Fig. 3, which involved a total simulation time of $t = 1.2$ day, were 208, 358, and 714 s for our proposed criterion (11), the mixed criterion (10), and the standard criterion (9), respectively. The corresponding total numbers of iterations were 2025, 4247, and 13048, respectively. In the sections below we shall make more comprehensive comparisons of the CPU times used by the different convergence criteria for various soil types, initial conditions, inlet boundary conditions, for infiltration in a layered soil, and for a two-dimensional flow problem.

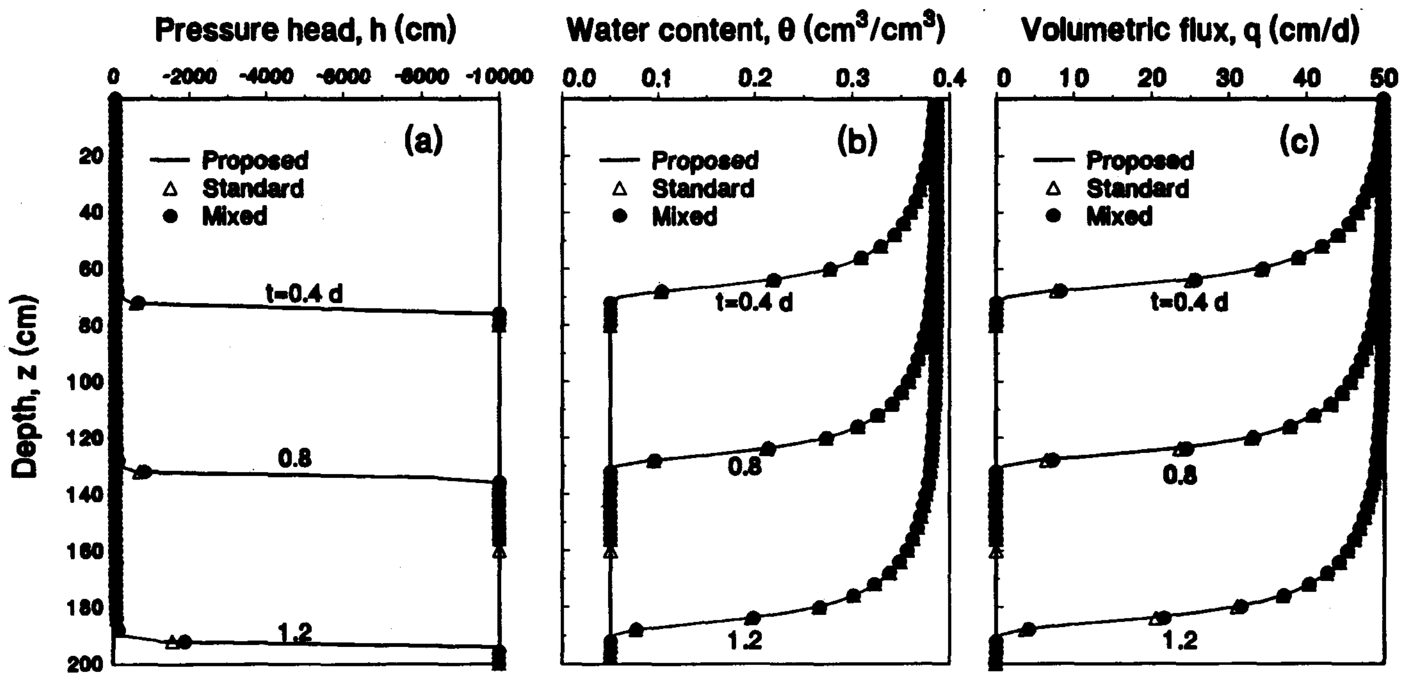

Fig. 3. Predicted pressure head (a), water content (b), and Darcian flux (c) profiles for the proposed, standard, and mixed convergence criteria assuming constant rate infiltration (50 cm day^{-1}) in a soil with $\theta_r = 0.05$, $\theta_s = 0.45$, $K_s = 100$ cm day^{-1}, $n = 5.0$, and $\alpha = 0.2$ cm^{-1} (Exp. 4, Table 1).

Table 1
CPU time and total number of iterations used by the proposed (11), mixed (10), and standard (9) convergence criteria for numerical experiments involving different types of soils

Exp. no.	Soil parameters		Boundary flux (cm day^{-1})	Initial pressure head (cm)	CPU time (s)			Total no. of iterations		
	α	n			Proposed	Mixed	Standard	Proposed	Mixed	Standard
1	0.015	1.5	$q_0 = 50$	−10000	42	44	62	2277	3661	5296
2	0.015	2.5	$q_0 = 50$	−10000	30	48	103	1765	1895	5917
3	0.200	4.0	$q_0 = 50$	−10000	128	336	466	2236	7106	9223
4	0.200	5.0	$q_0 = 50$	−10000	209	358	714	2025	4247	13048
5	0.200	6.0	$q_0 = 50$	−10000	208	–	–	3871	–	–
6	0.200	7.0	$q_0 = 50$	−10000	213	–	–	3934	–	–
7	0.200	9.0	$q_0 = 50$	−10000	237	–	–	4259	–	–
8	0.250	10.0	$q_0 = 50$	−10000	269	–	–	4501	–	–

–, Solution failed to converge.

5.1. Performance for different soil hydraulic characteristics

Fig. 4 presents the simulation results for ponded infiltration into two different soils, a relatively fine-textured soil ($\alpha = 0.015$ and $n = 1.5$), and a relatively coarse-textured soil ($\alpha = 0.2$ and $n = 5$), both having a uniform initial pressure distribution of $h_i = -10^4$ cm. Values for θ_r, θ_s, and K_s were the same as before. The three convergence criteria again produced essentially the same pressure head distributions at all times (Fig. 4). Very consistent solutions among the three convergence criteria were also found for the water content and the Darcian flux distributions (results not further presented here). However, some differences were observed in CPU time and total number of iterations. For the fine-textured soil (Fig. 4(a)), the computational requirements for the proposed nonlinear criterion (CPU time was 35 s and total number of iterations 2241) were comparable with those for the mixed criterion (34 s and 1901 iterations), but much less than those for the standard criterion (77 s and 5008 iterations). By comparison, the new criterion was found to be far more economical for the coarse-textured soil (Fig. 4(b)), for which the CPU times were 72, 240, and 500 s using the proposed, mixed, and standard criteria, respectively.

Very similar results were obtained for flux-controlled infiltration in different soils having the same initial condition (-10^4 cm) as before. As the nonlinear nature of the soil hydraulic properties is mostly represented in the values of α and n, we decided to vary only these two parameters while keeping the same θ_r (0.05), θ_s (0.45), and K_s (100 cm day^{-1}). Infiltration was assumed to occur at a rate of $q_0 = 50$ cm day^{-1} (i.e. one-half of K_s) at the soil surface. Our comparisons of CPU times for different convergence criteria always involved the same spatial discretization, initial time step, maximum number of iterations allowed during a particular time step, and total simulation time. Table 1 shows that CPU time and the total number of

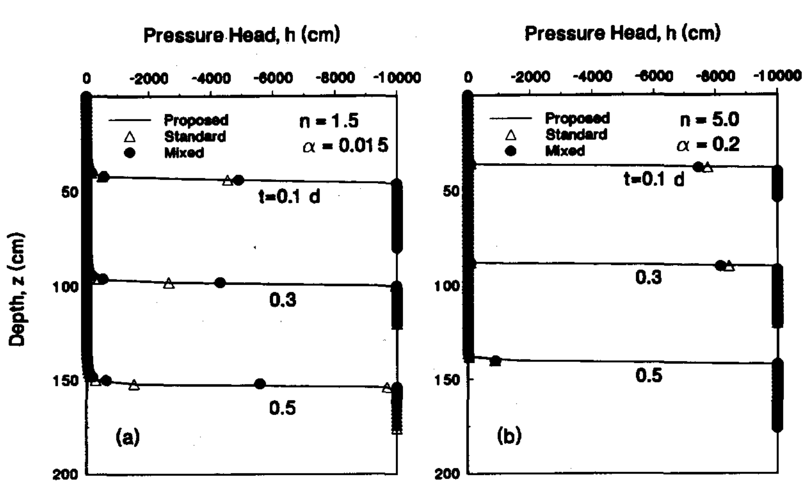

Fig. 4. Simulated pressure head distributions using the proposed, standard, and mixed convergence criteria for ponded infiltration ($h_0 = 0$) into (a) a relatively fine-textured soil ($n = 1.5$, $\alpha = 0.015$ cm^{-1}), and (b) a relatively coarse-textured soil ($n = 5.0$, $\alpha = 0.2$ cm^{-1}).

iterations for the three criteria generally increased with increasing values of α and n. However, the degree at which CPU time increased differed significantly among the three criteria. CPU time for the proposed criterion increased only little with n and/or α, whereas the CPU times for both the mixed and standard criteria increased dramatically. It should be noted from Table 1 that the CPU time and the total number of iterations were always smallest for the proposed nonlinear criterion, highest for the standard criterion, and intermediate for the mixed criterion.

Fig. 5 shows that improvements in computational efficiency of the proposed criterion were especially dramatic for relatively large n values typical of soils having relatively narrow pore-size distributions (mostly coarse-textured soils). Actually, the standard and mixed criteria failed to yield convergent solutions for $n > 5$. Fig. 6 presents predicted water content, pressure head, and volumetric flux distributions for a soil having extremely nonlinear soil hydraulic properties, i.e. $\alpha = 0.25$ cm^{-1} and $n = 10$. Numerical simulation of infiltration into such soils can be very difficult as shown by, among others, Huang et al. (1994). This example illustrates the robustness of the proposed criterion for flow problems involving highly nonlinear hydraulic properties.

5.2. Performance for different initial conditions

Accurate solutions for infiltration into dry soils are often difficult to obtain with standard numerical schemes (Zaidel and Russo, 1992) because of steep pressure head distributions and rapid advancement of the wetting front. Such problems usually require very small time increments and large numbers of iterations. We examined

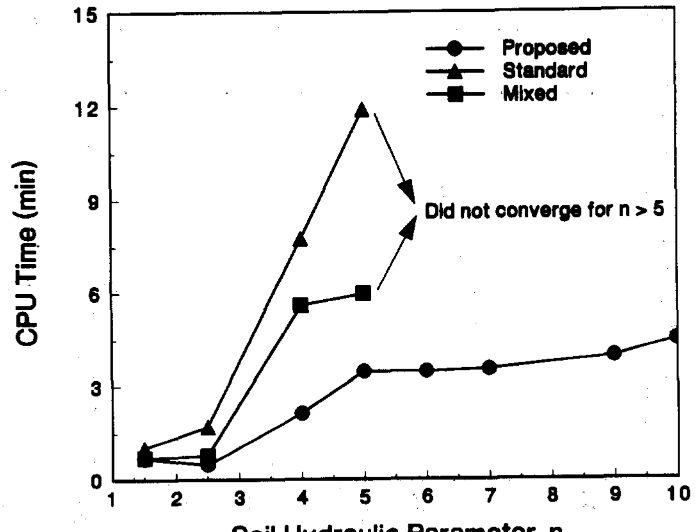

Fig. 5. CPU time vs. soil hydraulic parameter n for the numerical experiments listed in Table 1.

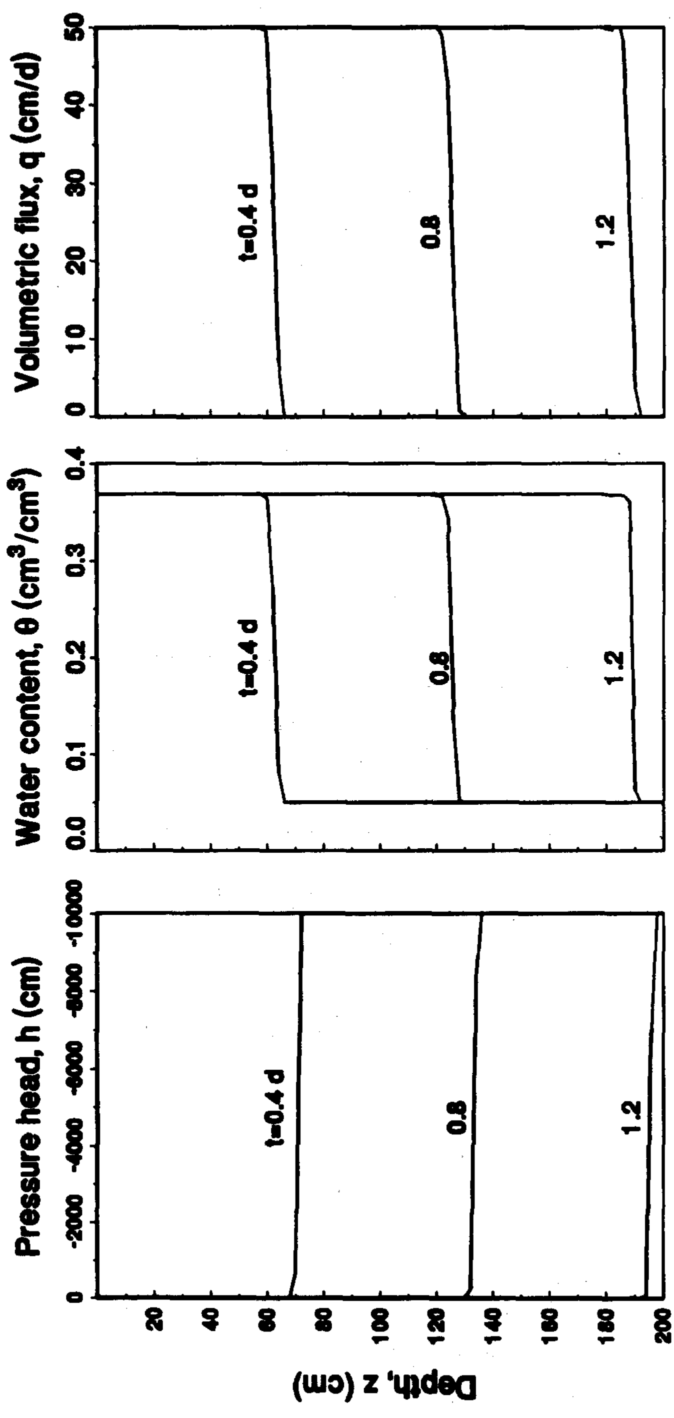

Fig. 6. Calculated pressure head, water content, and Darcian flux profiles obtained with the proposed convergence criterion for constant flux infiltration of 50 cm day^{-1} in a very coarse-textured soil with $n = 10$ and $\alpha = 0.25$ cm^{-1} (Exp. 8, Table 1).

Table 2
CPU time and total number of iterations used by the proposed (11), mixed (10), and standard (9) convergence criteria for numerical experiments involving different initial conditions

Exp. no.	Soil parameters		Boundary pressure head (cm)	Initial pressure head (cm)	CPU time (s)			Total no. of iterations		
	α	n			Proposed	Mixed	Standard	Proposed	Mixed	Standard
1	0.015	2.5	$h_0 = 0$	−1000	29	22	25	1763	1201	2277
2	0.015	2.5	$h_0 = 0$	−10 000	30	38	88	1765	3570	5917
3	0.015	2.5	$h_0 = 0$	−50 000	111	210	643	1994	4740	12858
4	0.015	2.5	$h_0 = 0$	−100 000	113	230	896	1978	5111	17229
5	0.015	2.5	$h_0 = 0$	−500 000	110	271	1795	1978	6130	36410
6	0.150	4.0	$h_0 = 0$	−1000	84	110	121	1393	2045	2139
7	0.150	4.0	$h_0 = 0$	−5000	84	165	266	1393	3158	4807
8	0.150	4.0	$h_0 = 0$	−10 000	84	192	358	1393	3588	6522
9	0.150	4.0	$h_0 = 0$	−50 000	84	259	855	1393	4889	15629

the performance of the proposed convergence criterion for infiltration in different soils under different initial conditions; results are summarized in Table 2. Two types of soils were selected: a medium-textured soil ($\alpha = 0.015$ and $n = 2.5$) and a relatively coarse-textured soil ($\alpha = 0.15$ and $n = 4.0$). The example simulated ponded infiltration with zero pressure head at the soil surface. Initial pressure heads ranged from -1000 cm of water to $-500\,000$ cm for the medium-textured soil, and from -1000 to $-50\,000$ cm for the coarse-textured soil. Figs. 7(a) and 7(b) show calculated pressure head profiles for the medium-textured soil having initial pressure heads of $h_i = -10^4$ cm and -10^5 cm, respectively. The three convergence criteria in both cases produced nearly identical solutions, but at the cost of significantly different computer times. For $h_i = -10^4$ cm, the standard criterion required about three times more CPU time than the proposed criterion (89 vs. 30 s). As the initial pressure head decreased (drier soil), the difference in computational efficiency between the standard and proposed criteria became even more pronounced: CPU time using the standard criterion (896 s) for $h_i = -10^5$ cm became eight times that of the proposed criterion (112 s). Except for the relatively wet initial condition ($h_i = -1000$ cm), CPU times for the mixed criterion were found to be between those needed for the proposed and the standard criteria. Although the CPU times generally increased with decreasing initial soil water pressure head (drier soils), the rates of increase were greatly different among the three convergence criteria (Figs. 8(a) and 8(b)), with the proposed criterion being the least sensitive to the value of h_i.

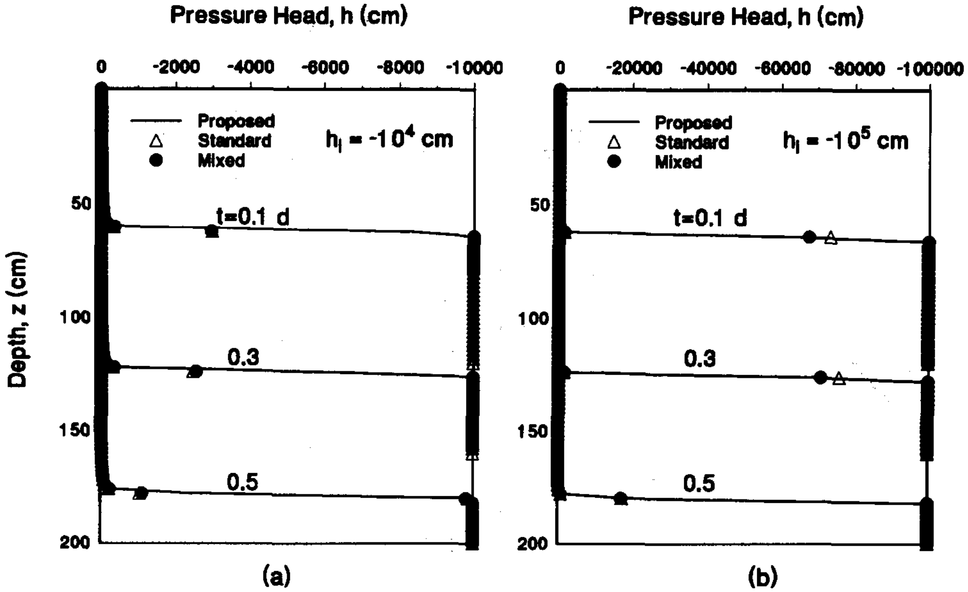

Fig. 7. Calculated pressure head profiles using the proposed, standard, and mixed convergence criteria for constant head infiltration ($h_0 = 0$) in a soil having $n = 2.5$ and $\alpha = 0.015$ cm^{-1} and with an uniform initial pressure head of (a) $h_i = -10^4$ cm and (b) $h_i = -10^5$ cm.

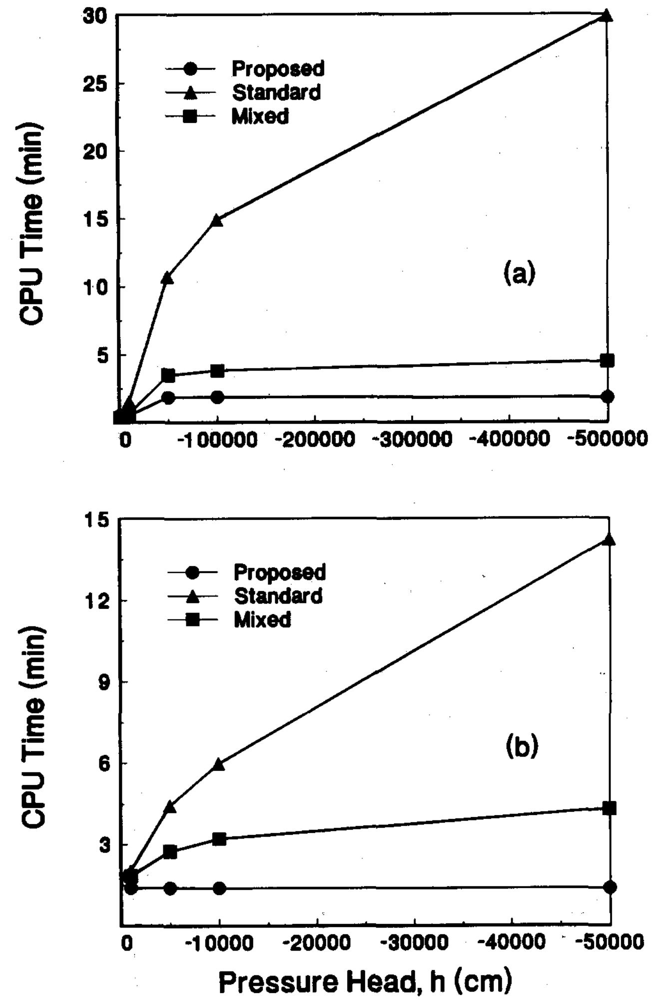

Fig. 8. CPU time vs. initial pressure head for the numerical experiments of Table 2 assuming (a) a loamy soil ($n = 2.5$, $\alpha = 0.015\ cm^{-1}$), and (b) a sandy soil ($n = 4.0$, $\alpha = 0.15\ cm^{-1}$).

These findings indicate a significant advantage of the proposed nonlinear convergence criterion over traditional criteria for infiltration problems involving extremely dry initial soil conditions.

5.3. Performance for a layered soil profile

The relative performance of the three convergence criteria for infiltration into a layered soil was also investigated. Numerical experiments were conducted for infiltration in a soil profile consisting of three distinct soil horizons: a relatively coarse-textured soil ($K_s = 100$ cm day^{-1}, $\theta_s = 0.4$, $\theta_r = 0.05$, $\alpha = 0.15$, $n = 4.0$) between 0 and 40 cm depth; a fine-textured soil ($K_s = 10$ cm day^{-1}, $\theta_s = 0.45$, $\theta_r = 0.05$, $\alpha = 0.015$, $n = 1.5$) between 40 and 100 cm; and a medium-textured soil ($K_s = 50$ cm day^{-1}, $\theta_s = 0.4$, $\theta_r = 0.05$, $\alpha = 0.015$, $n = 2.5$) between 100 and 200 cm. We assumed ponding with zero pressure head at the soil surface and a uniform initial pressure head of -10^5 cm. As for the homogeneous soil, calculated results for θ, h, and q were again essentially the same among the three different convergence criteria. Fig. 9 presents calculated pressure head distributions at three times. It should be noted that, as expected, a fully saturated zone developed in the upper coarse-textured soil overlying the fine-textured layer. The wetting front itself was always very steep because of the very dry initial condition. Numerical simulation for this example required approximately 8, 15, and 19 min for the proposed, mixed, and standard convergence criteria, respectively. We note here that, as compared with a homogeneous soil, numerical simulation of infiltration in a layered soil generally requires more CPU time, irrespective of the invoked convergence criterion. Several additional numerical experiments (not further reported here) for the same solution domain and

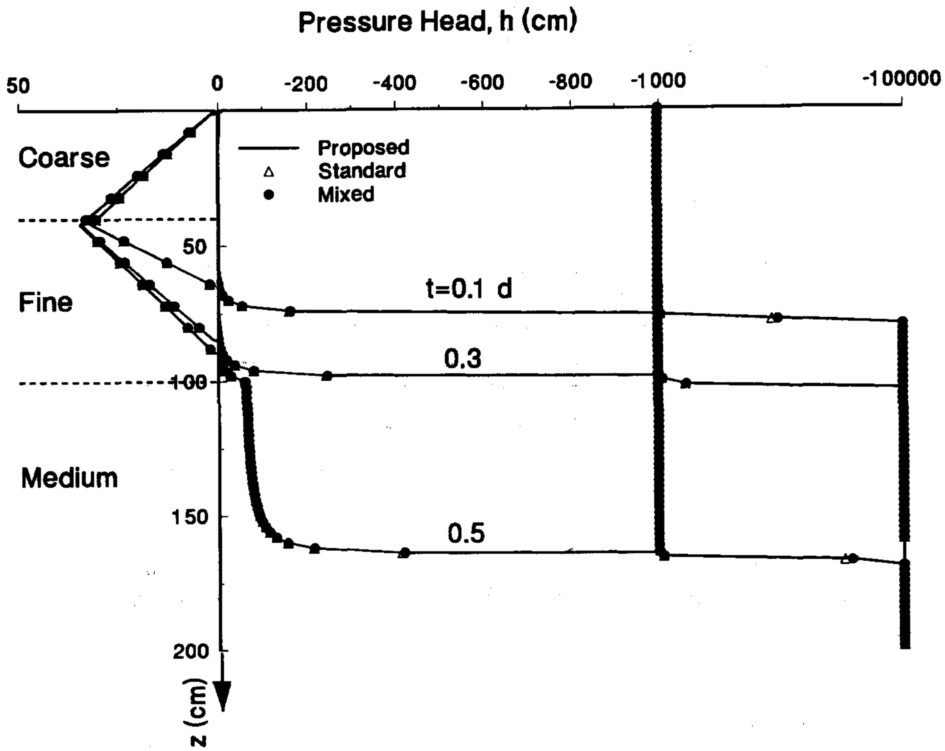

Fig. 9. Pressure head distributions calculated using the proposed, standard, and mixed convergence criteria for ponded infiltration ($h_0 = 0$) in a soil having three layers: a coarse-textured layer 1 (0–40 cm), a fine-textured layer 2 (40–100 cm), and a medium-textured layer 3 (note the different scales of the h-axis for different ranges in the pressure head).

the same total number of finite element nodes indicated that CPU time generally increased with the number of soil layers for all three convergence criteria. In each case, however, the new convergence criterion was found to require less computer time than the other two criteria.

The examples above show that the proposed convergence criterion always required the least amount of CPU time, irrespective of the type of boundary condition (flux or ponding) invoked at the soil surface. Numerical experiments were also conducted for different bottom boundary conditions, i.e. free draining and Dirichlet type conditions. Results of these simulations again indicated the superiority of the proposed nonlinear criterion as compared with the other two criteria (figures not further presented here). Results obtained thus far for the proposed convergence criterion always used a value of 0.0001 for δ_θ in (11). A large number of numerical experiments involving different hydraulic properties and initial and boundary conditions showed that CPU times could be further decreased somewhat, without appreciably affecting

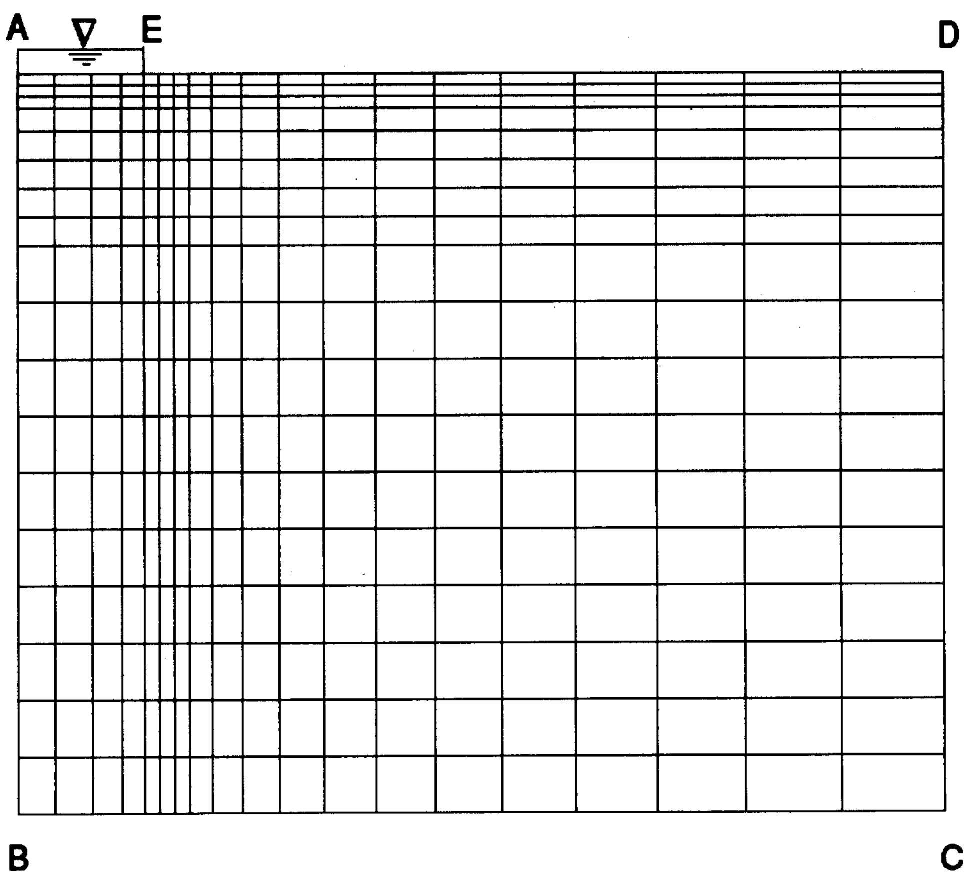

Fig. 10. Finite element mesh for the two-dimensional infiltration events. Zero-flux boundary conditions were used except as noted. The initial pressure head was -10^4 cm for all simulations.

the numerical accuracy, by increasing δ_θ to a value of about 0.001 depending upon the specific infiltration problem being simulated. Much higher values for δ_θ (e.g. 0.01 or higher) eventually produced inaccurate (mostly oscillating) results or even divergent solutions.

5.4. Performance for two-dimensional variably saturated flow

Computational efforts for multi-dimensional variably saturated flow problems should be far more demanding as compared with the one-dimensional case. The simulations presented below provide additional tests of the proposed convergence criterion for cases of flow in a vertical two-dimensional soil profile. The problem domain was taken to be of 125 cm width and 130 cm depth; the associated finite element mesh used for the ponded infiltration numerical experiment is illustrated in Fig. 10. All sides of the flow region were considered to be impervious, except for a strip of 17 cm length at the surface where ponded infiltration with zero pressure head was imposed. The solution domain was discretized into 342 quadrilateral elements involving 380 nodes. To minimize numerical errors, relatively small elements were implemented near the soil surface, with the size of elements gradually increasing with depth. Finer spatial increments were also implemented near the right edge of the ponding area where sharp gradients were expected to develop. Numerical simulations were carried out with the SWMS_2D code of Šimůnek et al. (1994), but properly modified to account for the different convergence criteria.

Both a layered and a homogeneous soil profile were considered for the two-dimensional problem. For the layered soil we considered a field soil profile in the Hupselse Beek watershed in the Netherlands (Šimůnek et al., 1994) consisting of two layers: a surface clayey soil layer (0–40 cm) and a subsurface loamy soil layer (40–130 cm). Soil hydraulic parameters of the two soil layers as estimated by Hopmans and Stricker (1989) are listed in Table 3. The invoked boundary conditions are listed in Table 3. We assumed a uniform initial pressure head ($h_i = -10^4$ cm) distribution across the profile. Numerical simulations were performed using both the standard and proposed convergence criteria given by (9) and (11), respectively. Fig. 11 shows contour plots of the pressure head after 72 h of infiltration. Calculated results for both criteria were found to be almost indistinguishable. However, the standard criterion

Table 3
Hydraulic parameters and boundary conditions for the two-dimensional flow experiment

	Hydraulic parameters		Boundary conditions
	Upper layer	Lower layer	
θ_s	0.399	0.339	$\left.\frac{\partial h}{\partial n}\right\|_{\mathrm{ABCDE}} = 0$
θ_r	0.0001	0.0001	
K_s (cm day^{-1})	29.8	45.4	
α (cm^{-1})	0.0174	0.0139	$h\|_{\overline{\mathrm{XE}}} = 0$
n	1.3757	1.6024	

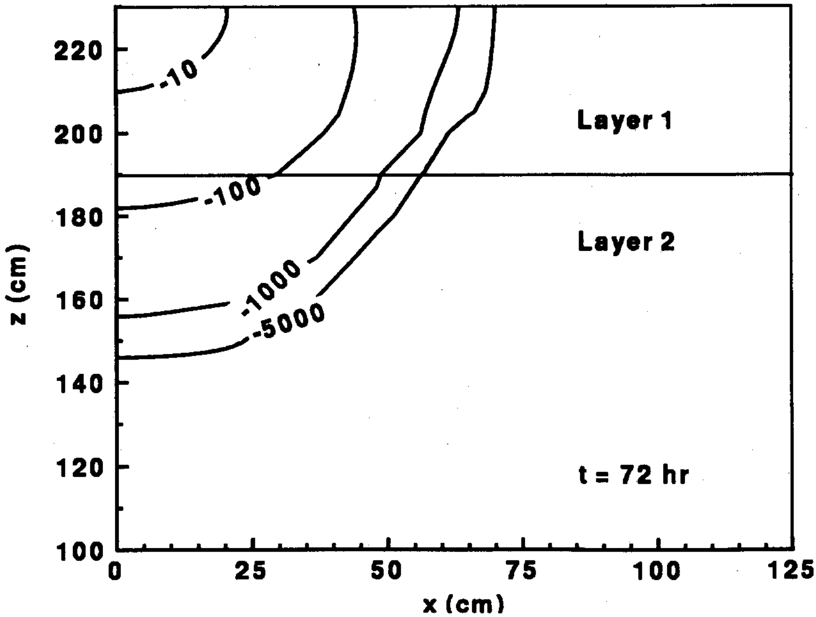

Fig. 11. Pressure head contours after 72 h of infiltration into a layered soil consisting of a fine-textured upper layer and a medium-textured lower layer, as calculated using the proposed criterion (continuous lines) and the standard criterion (dashed lines), respectively. Soil hydraulic properties are given in Table 3.

required more than twice as much CPU time (78 min) as the proposed criterion (37 min) for simulating the 3 day infiltration event.

We also simulated the same two-dimensional problem assuming a homogeneous soil profile, but with somewhat more nonlinear hydraulic properties: $\theta_r = 0.05$, $\theta_s = 0.45$, $K_s = 72$ cm day^{-1}, $n = 2.5$ and $\alpha = 0.1$ cm^{-1}. Initial and boundary conditions were the same as for the layered soil example. Calculations for the 4 h infiltration event used less than 1 h (54.5 min) of CPU time with the proposed criterion and 47.5 h with the standard criterion, indicating a more than 50 times improvement in efficiency for the proposed criterion. Several other tests, not further reported here, for two-dimensional flow using different soil hydraulic parameters produced similar findings of improved computational efficiency when the proposed nonlinear convergence criterion was adopted.

6. Summary and conclusions

A new nonlinear convergence criterion is proposed for the mixed-form algorithm of Celia et al. (1990) for solving the variably saturated flow equation. The nonlinear convergence criterion (11), derived using a Taylor series expansion of the water content $\theta^{n+1,m+1}$, consists of a term containing the absolute error of pressure head, and a term involving the soil water capacity. The proposed criterion was successfully applied to a large number of infiltration problems involving a variety of soil types, boundary conditions, initial conditions, homogeneous and layered soil profiles, and one- and two-dimensional flow problems. The performance of the proposed criterion was evaluated against a popularly used standard criterion involving the absolute error of pressure head only, and a mixed criterion consisting of absolute and relative errors. The following conclusions were drawn from our numerical experiments:

(1) although insuring perfect mass balance, the new criterion produced results which, for all numerical experiments, were very close to those obtained with the standard and mixed convergence criteria in terms of simulated water content, pressure head, and water flux distributions.

(2) Computational efforts (CPU time and total number of iterations) using the proposed criterion were always considerably less than those using the standard and mixed criteria for all scenarios tested.

(3) Reductions in computational effort using our proposed criterion were particularly significant for infiltration into relatively coarse-textured soils (high n and α values), infiltration in initially dry soils, and multidimensional infiltration problems.

(4) The proposed nonlinear criterion was found to be more robust than the standard and mixed criteria when the soil hydraulic characteristics were extremely nonlinear (high n and α) and/or when very dry initial soil conditions existed. Numerical solutions for these extreme conditions using the standard and mixed criteria failed to converge, or produced unstable and slowly convergent solutions (two-dimensional case).

We conclude that implementation of the proposed nonlinear convergence criterion will make the mixed-form algorithm of Celia et al. (1990) much more efficient and robust.

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