EFFICIENT AND ACCURATE NUMERICAL SCHEME FOR ONE-DIMENSIONAL INFILTRATION

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An efficient and accurate finite-difference scheme is presented for solving the one-dimensional Richards' equation. The numerical model is based on the 'mixed' form of Richards' equation which ensures the mass conservation. The Newton-Raphson scheme is incorporated in order to effectively handle the nonlinearity of the equation. An 'updating' coefficient is introduced to further enhance the convergence rate. The effect of the updating coefficient on the required number of iterations per time step was examined as well.

Keywords: infiltration, Richards' equation, finite difference.

1. INTRODUCTION

Richards' equation is the commonly accepted basis for detailed studies of water movement in saturated-unsaturated soils. Three standard forms of Richards' equation may be identified as the 'Ψ-based' form, the 'θ-based' form, and the 'mixed' (conservative) form. Solutions using the 'Ψ-based' formulation are known to produce unacceptably large mass balance errors[1], meanwhile the 'θ-based' formulation is not suitable for combined saturated-unsaturated flow or infiltration into layered soils[2]. The 'mixed' form of Richards' equation shows perfect mass balance in numerical calculation[1,3] and is applicable for all practical situations.

Numerous analytical and numerical solutions of Richards' equation have been developed over the past 30 years. Analytical solutions are applicable to highly simplified systems. They are not well suited for the more complex situations normally encountered in the field, but may prove to be useful for verification of numerical solutions. Of numerical calculations, the finite element techniques do not prove to have any advantage for one-dimensional simulations over the finite-difference techniques[1,4]. The finite-difference method , therefore, is frequently employed.

As Richards' equation is a nonlinear Fokker-Planck equation, proper linearization procedure has to be introduced. For this reason, the conventional iteration methods such as Newton-like and Picard method are widely used. For highly nonlinear problems, the Newton-Raphson method is known to be more efficient in computation than those methods[5,6].

From the viewpoint of efficiency of computation, accuracy of mass conservation, and flexible applicability to saturated-unsaturated problems, Richards' equation in the 'conservative' form is schematized by the finite-difference method, incorporating the Newton-Raphson scheme. Additionally, an 'updating' coefficient is introduced to further enhance the convergence rate of the Newton-Raphson scheme. Efficiency and accuracy of the proposed numerical scheme are quantified by making direct comparison with existing numerical methods.

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2. THEORY

The one-dimensional continuity equation is given by

$$\partial\theta/\partial t = -\partial q/\partial z \quad \cdots\cdots (1)$$

The flux of water q is expressed as Darcy's law:

$$q = -K(\partial\Psi/\partial z - 1) \quad \cdots\cdots (2)$$

where $\Psi(z,t)$ is the pressure head; $\theta(\Psi)$ the volumetric moisture content; $K(\Psi)$ the hydraulic conductivity; t the time; z the depth oriented positively downward.

Combining Eqs. (1) and (2) yields the one-dimensional Richards' equation in the 'mixed' form:

$$\partial\theta/\partial t = \partial[K(\partial\Psi/\partial z - 1)]/\partial z \quad \cdots\cdots (3)$$

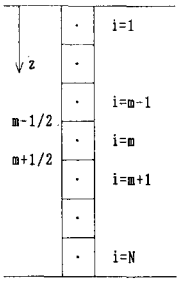

Fig. 1. Finite-difference grid.

Approximate finite-difference form of Eq. (1) for a typical cell m (Fig. 1) at time $t^n + \omega\Delta t$, where $0 \leqq \omega \leqq 1$, is given by

$$(\theta_m^{n+1} - \theta_m^n)/\Delta t = -(q_{m+1/2} - q_{m-1/2})/\Delta z \quad \cdots\cdots (4)$$

where θ_m denotes the moisture content of cell m; $q_{m+1/2}$ and $q_{m-1/2}$ the average fluxes across the interfaces m+1/2 and m-1/2 during the time step Δt, respectively; Δz the nodal spacing; $\Delta t = t^{n+1} - t^n$ the time step; n previous time level; n+1 current time level.

The average flux over the period Δt across the interface m+1/2 may be determined as

$$q_{m+1/2} = \omega q_{m+1/2}^{n+1} + (1-\omega)q_{m+1/2}^n \quad \cdots\cdots (5)$$

where ω is a time-weighting coefficient, ω = 0, 0.5, and 1 coresponds to the explicit, Crank-Nicolson, and implicit schemes, respectively.

The finite-difference form of Eq. (2) written at the interface m+1/2 is

$$q_{m+1/2} = -K_{m+1/2}[(\Psi_{m+1} - \Psi_m)/\Delta z - 1] \quad \cdots\cdots (6)$$

Substituting Eqs. (5) and (6) into Eq. (4), one obtains

$$\omega\Delta t/\Delta z^2 [-K_{m+1/2}^{n+1}(\Psi_{m+1}^{n+1} - \Psi_m^{n+1} - \Delta z) + K_{m-1/2}^{n+1}(\Psi_m^{n+1} - \Psi_{m-1}^{n+1} - \Delta z)]$$
$$+ \theta_m^{n+1} - \theta_m^n + (1-\omega)\Delta t/\Delta z [q_{m+1/2}^n - q_{m-1/2}^n] = 0 \quad \cdots\cdots (7)$$

Since K and θ are nonlinear functions of Ψ, Eq. (7) needs to be linearized. Denoting the left-hand side of Eq. (7) as a function R, Taylor expansion of Eq. (7) about an assumed solution yields

$$R^{n+1,r+1} = R^{n+1,r} + \Sigma\,\partial R/\partial\Psi_j\Big|^{n+1,r}\delta\Psi_j = 0 \quad \cdots\cdots (8)$$

where j = m-1, m and m+1; r denotes the iteration level; $\delta\Psi = \Psi^{n+1,r+1} - \Psi^{n+1,r}$ are the unknowns to progress from the known values at iteration r to the next unknown values at iteration r+1 at the same time level n+1.

Using the arithmetic average for the internodal hydraulic conductivities, the linearized form of Eq. (8) written for a particular cell m (Fig. 1) is given by

$$E_m^{n+1,r}\delta\Psi_{m-1} + F_m^{n+1,r}\delta\Psi_m + G_m^{n+1,r}\delta\Psi_{m+1} + H_m^{n+1,r} = 0 \quad \cdots\cdots (9)$$

where

$$E_m^{n+1,r} = -\omega\Delta t/\Delta z^2 [K_{m-1/2}^{n+1,r} - D_{m-1}^{n+1,r}(\Psi_m^{n+1,r} - \Psi_{m-1}^{n+1,r} - \Delta z)/2] \quad \cdots\cdots (10)$$

$$F_m^{n+1,r} = C_m^{n+1,r} + \omega\Delta t/\Delta z^2 [K_{m-1/2}^{n+1,r} + D_m^{n+1,r}(\Psi_m^{n+1,r} - \Psi_{m-1}^{n+1,r} - \Delta z)/2$$
$$+ K_{m+1/2}^{n+1,r} - D_m^{n+1,r}(\Psi_{m+1}^{n+1,r} - \Psi_m^{n+1,r} - \Delta z)/2] \quad \cdots\cdots (11)$$

$$G_m^{n+1,r} = -\omega\Delta t/\Delta z^2 [K_{m+1/2}^{n+1,r} + D_{m+1}^{n+1,r}(\Psi_{m+1}^{n+1,r} - \Psi_m^{n+1,r} - \Delta z)/2] \quad \cdots\cdots (12)$$

$$H_m^{n+1,r} = \theta_m^{n+1,r} - \theta_m^n + (1-\omega)\Delta t/\Delta z\,(q_{m+1/2}^n - q_{m-1/2}^n)$$
$$+ \omega\Delta t/\Delta z^2\,[K_{m-1/2}^{n+1,r}(\Psi_m^{n+1,r} - \Psi_{m-1}^{n+1,r} - \Delta z) - K_{m+1/2}^{n+1,r}(\Psi_{m+1}^{n+1,r} - \Psi_m^{n+1,r} - \Delta z)] \quad \cdots\cdots (13)$$

where $C = \partial\theta/\partial\Psi$ is the specific moisture capacity; $D = dK/d\Psi$ the derivative of the hydraulic conductivity with respect to pressure head.

Eq. (9) expresses the exact mass conservation of cell m in finite-difference form as $\delta\Psi_{m-1}$, $\delta\Psi_m$ and $\delta\Psi_{m+1}$ approach zero. If we simply assign Ψ^n to $\Psi^{n+1,0}$ in Eq. (9) at the start of each new time step (r = 0) as has been commonly done, the following equation is obtained;

$$H_m^{n+1,0} = \Delta t/\Delta z(q_{m+1/2}^n - q_{m-1/2}^n) \neq 0 \quad \cdots\cdots (14)$$

As H is required to approach zero in order to obtain a converged solution, an 'updating' coefficient η will be introduced at the start of each new time step. Since the Newton-Raphson iterative scheme is strongly convergent (second-order convergence rate), appropriate estimation of initial solutions could further enhance the convergence rate.

The discretization procedure involved yields the following iterative algorithm for advancing the approximate solution from time $t = n\Delta t$ to time $t = (n+1)\Delta t$.

Step 1: Let n + 1 be replaced by n, and at the first iteration level (r = 0) the value of $\Psi_m^{n+1,0}$ is set by $\Psi_m^n + \eta(\Psi_m^n - \Psi_m^{n-1})$, in case of infiltration $\Psi_{m+1}^{n+1,0} < \Psi_m^{n+1,0}$.

Step 2: Compute the residual $H_m^{n+1,r}$.

If $\max|H_m^{n+1,r}| < \varepsilon$, then accept the values of $\Psi_m^{n+1,r}$. Go to step 1.

Step 3: Compute the coefficients of Eq. (9), then solve for $\delta\Psi_m$.

Step 4: Let $\Psi_m^{n+1,r} + \delta\Psi_m \rightarrow \Psi_m^{n+1,r+1}$, then go to step 2.

In the preceding equations, m = 1 to N, in which N is the number of cells in the considered domain, and $\varepsilon = 10^{-5}$ (L^3/L^3) the convergence tolerance.

3. ILLUSTRATIVE EXAMPLES

The soil characteristics, initial and boundary conditions, discretization parameters, and convergence tolerance used by Cooley[7] and Celia et al.[1] are summarized in Table 1. For the purpose of direct comparison, those parameters were employed in the present simulation if not specified otherwise. The nodes in the proposed scheme are centered in cells (Fig. 1), and hence only the second half of the first cell is included in the flow domain.

Table 1. Calculation conditions.

Example 1: Cooley[7]	Example 2: Celia et al.[1]
$\theta = \theta_s(5.4/\lvert\Psi\rvert)^{0.2}$ $\Psi \leqq -5.4$ cm	$\theta(\Psi) = \theta_r + \dfrac{\theta_s - \theta_r}{[1 + (\alpha\lvert\Psi\rvert)^n]^m}$
$K = K_s(5.4/\lvert\Psi\rvert)^{2.6}$ $\Psi \leqq -5.4$ cm	$K(\Psi) = K_s \dfrac{\{1 - (\alpha\lvert\Psi\rvert)^{n-1}[1 + (\alpha\lvert\Psi\rvert)^n]^{-m}\}^2}{[1 + (\alpha\lvert\Psi\rvert)^n]^{m/2}}$
$\theta = \theta_s = 0.52$ $\Psi \geqq -5.4$ cm	$\alpha = 0.0335$, $n = 2$, $m = 1 - 1/n$
$K = K_s = 3.125$ cm/hr $\Psi \geqq -5.4$ cm	$\theta_s = 0.368$, $\theta_r = 0.102$, $K_s = 0.00922$ cm/s
$\Psi(z,t=0) = -130.54$ cm	$\Psi(z,t=0) = -1000$ cm
$\Psi(z=0,t)0) = -5.4$ cm	$\Psi(z=0,t)0) = -75$ cm
$\Psi(z=49,t)0) = -130.54$ cm	$\Psi(z=70,t)0) = -1000$ cm
Length of column L = 49 cm	Length of column L = 70 cm
$\Delta z = 1$ cm, $\Delta t = 0.1$ hr	$\Delta z = 2.5$ cm, $\Delta t = 100$ s, 3600 s
Convergence tolerance $\varepsilon = 0.001$(cm)	Convergence tolerance $\varepsilon = 10^{-8}$(sec^{-1})
Time-weighting coefficient $\omega = 1$	Time-weighting coefficient $\omega = 1$

(a). Example 1 (One-Dimensional Vertical Infiltration into Moderately Dry Soil)

This example was used as one of the simulations by Cooley[7], in which a subdomain finite element technique was employed to solve the Ψ-based Richards' equation. Cooley[7] developed an empirical relaxation scheme for updating nodal pressure head values to enhance the convergence rate. His scheme was later adopted by Huyakorn et al.[8] and Kaluarachchi and Parker[9].

Fig. 2 presents the profiles of moisture content normalized by the saturated moisture content obtained by Cooley[7] and our simulation. At time 1.2 hr, Cooley's[7] results lag slightly behind the present results, but at time 3.05 hr the difference increases considerably. Fig. 3 reveals that at time 1.2 hr the final shape of the front has already established. In this case, the theoretical downward velocity of the front corresponding to a hydraulic gradient of unity is $K_s/(0.52 - 0.275) = 12.755$ cm/hr, where 0.52 is the saturated moisture content and 0.275 is the initial moisture content. The computed velocity given by Cooley[7] is 12.432 cm/hr which is 2.53 % lower than the theoretical velocity. The computed velocity by our simulation is 23.75 cm/(3.05-1.2) hr = 12.838 cm/hr which is 0.65 % higher than the theoretical velocity. This comparison demonstrates that the results obtained by the present method is more accurate than those by Cooley's model[7]. In our calculation, the mass balance error MBE, which is defined as

$$MBE = |W_{cum} - W_{ch}| / W_{cum} \quad \cdots\cdots (15)$$

is less than 1×10^{-6}, where W_{cum} is the net cumulative flux into the computed domain; W_{ch} the change of water in the computed domain.

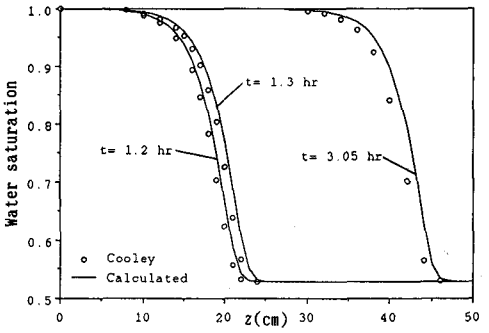

Fig. 2. Comparison of water saturation profiles computed by Cooley and our simulation.

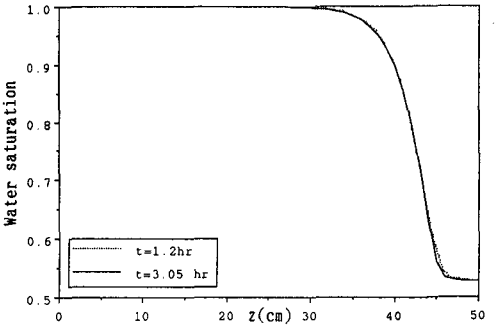

Fig. 3. Collapse of water saturation profiles by shifting the 1.2 hr profile a distance of 23.75 cm.

Fig. 4 presents the number of iterations per time step required in the present model and the effect of the updating coefficient η upon the convergence rate. It must be noted that Cooley's[7] model required at least 53 iterations per time step.

This large difference in number of iterations between the two models could be explained: (1) the derivatives of hydraulic conductivity with respect to pressure head were ignored in Cooley's model[7], as the result the theoretical second-order rate of convergence was lost; (2) for the Ψ-based form of Richards' equation, more iterations per time step is required to obtain the same convergence tolerance than those required by the 'mixed' form. This may be due to the difficulty in evaluating the appropriate specific capacity terms in the Ψ-based form of Richards' equation to guarantee the mass balance.

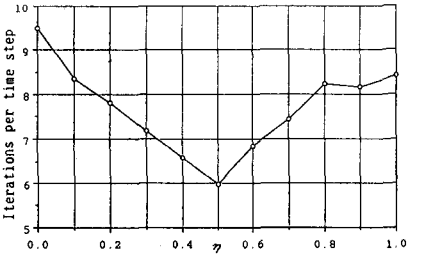

Fig. 4. Effect of the updating coefficient η upon the convergence rate.

(b). Example 2 (One-Dimensional Vertical Infiltration into Dry Soil)

The numerical simulation of infiltration into very dry soils is of considerable interest. Because the strong nonlinearity of functions $K(\Psi)$ and $\theta(\Psi)$ as well as the very steep wetting front render usually the solution difficult to be obtained.

Celia et al.'s[1] model is termed as the modified Picard or Newton-like scheme. They used the 'mixed' form of Richards' equation, but ignored the derivatives of the hydraulic conductivity with respect to pressure head.

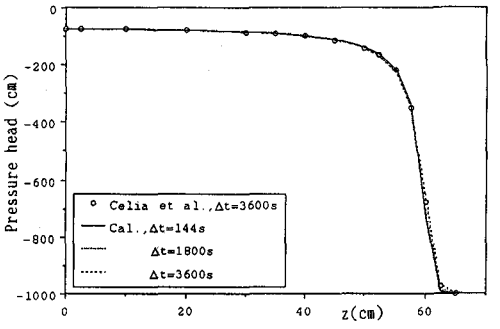

Fig. 5. Comparison of pressure head profiles computed by Celia et al. and our simulation at time t = 24 hr.

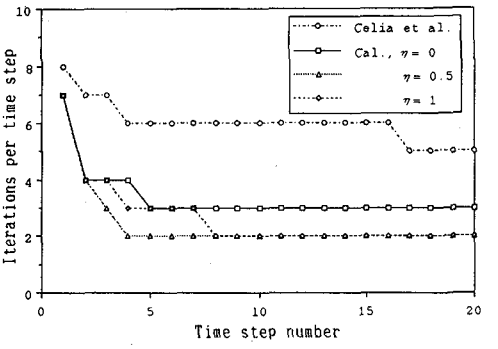

Fig. 6. Number of iterations per time step for Δt= 100s required by Celia et al.'s method and our simulation.

As shown in Fig. 5, there exists good agreement in the pressure head profiles between Celia et al.'s[1] and our result, keeping the mass balance error MBE less than $1x10^{-5}$ in our simulation. It appears that for infiltration into dry soils the time step does not have large influence on the shape of the wetting front as long as the solution for each time step is converged. A similar observation was reported by Kabala and Milly[10]. On the other hand, for infiltration into wet soils, the wetting front diffuses more as a time step Δt increases (the results are not shown here due to space limitation). In Fig. 6, the number of iterations required per time step during the first 20 time steps is plotted. The simulation was carried out using Δt = 100 s and a convergence tolerance of $\varepsilon = 10^{-8}$ (sec^{-1}) as used by Celia et al.[1]. In our simulations, a minimum of two iterations per time step was employed in order to obtain a stable numerical solution. This figure demonstrates that the Newton-Raphson method is more effective in convergence than the method used by Celia et al.[1].

Fig. 7 presents the effect of the updating coefficient η upon the convergence rate. All simulations were carried out under the conditions Δz = 2.5 cm and a constant convergence tolerance of $\varepsilon = 10^{-5}$ (L^3/L^3). Fig. 8 presents the same results normalized by the number of iterations calculated with coefficient η = 0. It can be seen that the coefficient η does not have large influence on the convergence rate for small values of Δt. This is due to the fact that only 2 or 3 iterations per time step are required so as to obtain a converged solution. However, it is apparent that the coefficient η improves substantially the convergence rate when Δt is larger.

4. CONCLUSIONS

1. As has been observed by Allen and Murphy[3], for the Ψ-based form there seems to be no simple method of choosing the time level between the interval $[n\Delta t, (n+1)\Delta t]$ to estimate the value of the specific capacity terms which guarantee the global mass balance. For this reason, Kaluarachchi and Parker[9] investigated various means of determining the specific capacity terms and their effects on the mass balance accuracy. Meanwhile, Huyakorn et al[5] proposed a chord-slope method to evaluate the specific capacity terms. In this study, the conservative form of Richards' equation, which ensures the mass balance, is used to circumvent such a difficulty.

2. The transformed Richards' equation such as the hyperbolic sine transform[11] appears to provide no additional advantage in simulating infiltration into dry soil, because this

particular situation can be simulated accurately by the conservative form of Richards equation.

3. The Newton-Raphson scheme for solving the conservative form of Richards' equation is more efficient in computation than the Newton-like or modified-Picard schemes.

4. The effect of the updating coefficient η on the convergence rate is strongly influenced by time step, nodal spacing and initial conditions, and weakly affected by soil characteristics and boundary-condition types. It is, thus, difficult to define an optimized value of the updating coefficient. However, η = 0.5 may be used to at least enhance the convergence rate of the proposed scheme.

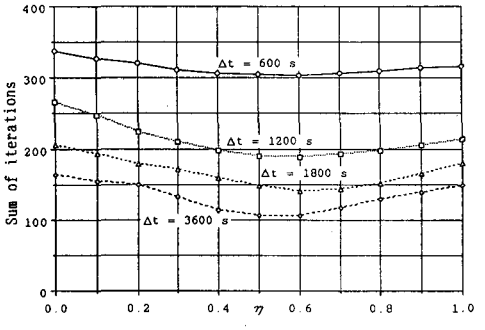

Fig. 7. Effect of the updating coefficient η upon the convergence rate, sum of iterations evaluated at time t = 24 hr.

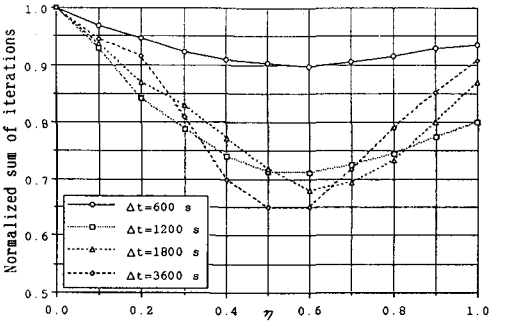

Fig. 8. Relation between normalized sum of iterations and the updating coefficient η.

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