Comparison of Finite Difference Schemes for Water Flow in Unsaturated Soils

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Abstract—Flow movement in unsaturated soil can be expressed by a partial differential equation, named Richards equation. The objective of this study is the finding of an appropriate implicit numerical solution for head based Richards equation. Some of the well known finite difference schemes (fully implicit, Crank Nicolson and Runge-Kutta) have been utilized in this study. In addition, the effects of different approximations of moisture capacity function, convergence criteria and time stepping methods were evaluated. Two different infiltration problems were solved to investigate the performance of different schemes. These problems include of vertical water flow in a wet and very dry soils. The numerical solutions of two problems were compared using four evaluation criteria and the results of comparisons showed that fully implicit scheme is better than the other schemes. In addition, utilizing of standard chord slope method for approximation of moisture capacity function, automatic time stepping method and difference between two successive iterations as convergence criterion in the fully implicit scheme can lead to better and more reliable results for simulation of fluid movement in different unsaturated soils.

Keywords—Finite Difference methods, Richards equation, fully implicit, Crank-Nicolson, Runge-Kutta.

I. INTRODUCTION

PREDICTION of infiltration or fluid movement in the unsaturated soils is an important problem in different field of science and engineering. One of the most important environmental problems is the transfer of the different pollutant (e.g. pesticides) from ground surface to groundwater through the unsaturated zone. The vertical water flow in unsaturated soil is simulated by combination of Darcy's law and mass conservation equation, yielding the Richards equation that can be expressed as different forms. Equation (1) shows the head based (h-based) form of Richards equation.

$$C(h)\frac{\partial h}{\partial t} - \nabla.K(h)\nabla h + \frac{\partial K}{\partial z} = 0 \qquad (1)$$

Where h[L] is pressure head, $C(h) = \frac{d\theta}{dh}[\frac{1}{L}]$ is specific moisture capacity, $\theta[\frac{L^3}{L^3}]$ is moisture content, $K(h)[\frac{L}{T}]$ is unsaturated hydraulic conductivity, t[T] is the time and z[L] is the vertical dimension (assumed positive downward).

Reference [1] compared six finite difference (FD) schemes to solve one-dimensional Richards equation. They compared the calculated and measured infiltration profiles in a sandy soil. Their results showed the close agreement between observed water content profiles and those computed with different numerical schemes, as well as the close agreement among these six schemes indicate that the numerical methods are reliable tools for prediction of infiltration of water into the soil. In addition, the excellent agreement between the implicit approximation and Philip's quasi-analytical solution showed that the numerical methods can yield accurate results.

Reference [2] used fully implicit (Backward Euler) with Picard iteration method for solving the h-based form of Richards equation. The results showed poor mass balance of h-based form. Reference [3] demonstrated that efficient mass conservative solution of h-based form of Richards equation can be obtained using the appropriate methods for evaluation of the moisture capacity function. The h-based form employing standard chord slop (SCS) approximation of moisture capacity showed excellent mass balance results [3].

The objective of this study is to investigate the performance of various implicit FD schemes (fully implicit, Crank-Nicolson and Runge-Kutta) for numerical approximation of h-based Richards equation. In addition, the effects of various convergence criteria, time stepping methods and approximations of moisture capacity are evaluated and the best FD method for solution of h-based Richards equation is determined.

II. FINITE DIFFERENCE APPROXIMATIONS

The FD schemes that are discussed in this study are consist of fully implicit, Crank-Nicolson (C-N) and Runge-Kutta (One step-two stage method). The Pichard linearization method is applied for linearization of k and C coefficients.

The general discretized form of Richards equation after discretization, linearization and simplification can be expressed as (2).

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$$A\,h_{i-1}^{n+1,m+1} + B\,h_i^{n+1,m+1} + D\,h_{i+1}^{n+1,m+1} = E \qquad (2)$$

Where, $h_i^{n+1,m+1}$ is the pressure head value in the node i at time level n+1 and iteration stage m+1. The coefficients A, B, D and E have different expressions in the numerical schemes. Tables I and II show the expression of these coefficients for different FD schemes. In these tables, the Δz is constant spacing, Δt is the time step, $k_i^{n+1,m}$, $C_i^{n+1,m}$ and $\theta_i^{n+1,m}$ are the hydraulic conductivity, moisture capacity and moisture content in node i at time level n+1 in iteration stage m. h_i^n is the pressure head in node i and at time level n. k_i^* and C_i^* are $k(h_i^*)$ and $C(h_i^*)$, respectively which h_i^* can be calculated by (3):

$$h_i^* = \frac{\Delta t}{4 \times C_i^n}\left[\frac{k_{i+1}^n + k_i^n}{2} \times \frac{h_{i+1}^n - h_i^n}{\Delta z^2} - \frac{k_i^n + k_{i-1}^n}{2}\right.$$
$$\left. \times \frac{h_i^n - h_{i-1}^n}{\Delta z^2} - \frac{k_{i+1}^n - k_i^n}{2 \times \Delta z}\right] + h_i^n \qquad (3)$$

Where, k_i^n, C_i^n and h_i^n are the hydraulic conductivity, moisture capacity and pressure head in the node i and at the time level n.

TABLE I
A AND B COEFFICIENTS FOR DIFFERENT SCHEMES

Scheme	A	B
Fully implicit	$-\dfrac{k_i^{n+1,m} + k_{i-1}^{n+1,m}}{2\,\Delta z^2}$	$\dfrac{C_i^{n+1,m}}{\Delta t} + \dfrac{k_{i+1}^{n+1,m} + 2k_i^{n+1,m} + k_{i-1}^{n+1,m}}{2\,\Delta z^2}$
Crank-Nicolson	$-\dfrac{k_i^{n+1,m} + k_{i-1}^{n+1,m}}{4\,\Delta z^2}$	$\dfrac{C_i^{n+1,m}}{\Delta t} + \dfrac{k_{i+1}^{n+1,m} + 2k_i^{n+1,m} + k_{i-1}^{n+1,m}}{4\,\Delta z^2}$
Runge-Kutta	$\dfrac{-k_i^{n+1,m} + k_{i-1}^{n+1,m}}{6\Delta z^2}$	$\dfrac{C_i^{n+1,m}}{\Delta t} + \dfrac{k_{i+1}^{n+1,m} + 2k_i^{n+1,m} + k_{i-1}^{n+1,m}}{6\Delta z^2}$

A. Approximations of Specific Moisture Capacity

The approximation of C (specific moisture capacity) can be performed by two different methods. The first method is the estimation of C by analytical derivation of $\theta(h)$, which is named tangent approximation. The second method is standard chord slope (SCS) approximation [3]. The SCS method is expressed by (5).

$$C_i^n = \frac{D_t\theta_i^n}{D_t h_i^n} = \frac{\theta_i^{n+1} - \theta_i^n}{h_i^{n+1} - h_i^n} \qquad (5)$$

In this study, the tangent and SCS approximations are utilized for approximation of C with various FD schemes and the results of tangent and SCS methods are compared.

TABLE II
D AND E COEFFICIENTS FOR DIFFERENT SCHEMES

Scheme	D	E
Fully implicit	$-\dfrac{k_i^{n+1,m} + k_{i+1}^{n+1,m}}{2\,\Delta z^2}$	$\dfrac{-k_{i+1}^{n+1,m} + k_{i-1}^{n+1,m}}{2\Delta z} + C_i^{n+1,m}\dfrac{h_i^n}{\Delta t}$
Crank-Nicolson	$-\dfrac{k_i^{n+1,m} + k_{i+1}^{n+1,m}}{4\,\Delta z^2}$	$\dfrac{-k_{i+1}^{n+1,m} + k_{i-1}^{n+1,m}}{2\Delta z} + C_i^{n+1,m}\dfrac{h_i^n}{\Delta t} + [\dfrac{k_{i+1}^{n+1,m} + k_i^{n+1,m}}{2} \times (h_{i+1}^n - h_i^n) - \dfrac{k_{i-1}^{n+1,m} + k_i^{n+1,m}}{2} \times (h_i^n - h_{i-1}^n)]/(2\Delta z^2)$
Runge-Kutta	$\dfrac{-k_i^{n+1,m} + k_{i+1}^{n+1,m}}{6\Delta z^2}$	$\dfrac{-k_{i+1}^{n+1,m} + k_{i-1}^{n+1,m}}{6\Delta z} + \dfrac{C_i^{n+1,m} \times h_i^n}{\Delta t} + \dfrac{2C_i^{n+1,m}}{3C_i^*} \times [\dfrac{(k_{i+1}^* + k_i^*)(h_{i+1}^* - h_i^*)}{2\,\Delta z^2} - \dfrac{(k_{i-1}^* + k_i^*)(h_i^* - h_{i-1}^*)}{2\,\Delta z^2} + \dfrac{(-k_{i+1}^* + k_{i-1}^*)}{2\,\Delta z}]$

B. Convergence Criterion

In the iterative methods (e.g. Picard method), the iterative process continues until the difference between the calculated pressure heads between two successive iteration levels in each node becomes less than a predefined tolerance (δa) as shown in (6).

$$\left| h^{n+1,m+1} - h^{n+1,m} \right| \le \delta a \qquad (6)$$

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Although it is true that more accurate solution can be obtained with smaller values of tolerance, but the computational time increases. δa is widely varying, for instance $\delta a = 0.01$ cm adopted for simulation three dimensional flow in unsaturated soil using finite element scheme [4] but δa =1cm used for drainage simulation [4]. In this study, $\delta a = 0.1$ cm has been adopted.

The second convergence criterion suggests to use of the entire storage term ($C^{n+1,m}\left|h_i^{n+1,m+1} - h_i^{n+1,m}\right|$) instead of the absolute error ($h_i^{n+1,m+1} - h_i^{n+1,m}$); therefore the second convergence criterion can be expressed as (7).

$$C^{n+1,m}\left|h_i^{n+1,m+1} - h_i^{n+1,m}\right| = \left|\theta^{n+1,m+1} - \theta^{n+1,m}\right| \le \delta_\theta \qquad (7)$$

δ_θ has no a distinct value. Reference [5] used of $\delta_\theta = 0.0001$ and in this study, δ_θ is considered equal to 0.0001.

The third suggested convergence criterion is the use of an empirical convergence criterion, which involves both absolute error (δa) and relative error (δr) as presented in (8).

$$\left|h^{n+1,m+1} - h^{n+1,m}\right| \le \delta r \left|h^{n+1,m+1}\right| + \delta a \qquad (8)$$

The adopted values for the relative tolerance (δr) have ranged from 0.001 to 0.01, depending upon the desired accuracy. In this study, $\delta r = 0.001$ has been adopted.

The performance of various convergence criteria is evaluated for fully implicit and C-N methods but the standard tolerance method (δa) has been used for Runge-Kutta method.

C. Time Step

In the numerical methods, the time step cab be predefined which is named constant time stepping. Another approach is the automatic time stepping. Equation (9) presents the automatic time stepping method.

$$\text{If } N \le 3 \text{ then } \Delta t^{new} = \mu_1 \Delta t^{old}$$
$$\text{If } 3 < N < 7 \text{ then } \Delta t^{new} = \Delta t^{old} \qquad (9)$$
$$\text{If } 7 \le N \le N_{max} \text{ then } \Delta t^{new} = \mu_2 \Delta t^{old}$$
$$\text{If } N_{max} < N \text{ then } \Delta t^{new} = \frac{\Delta t^{old}}{3}$$

Which N is the iteration number in each stage, N_{max} is the maximum number of iterations that its range is from 10 to 50. Δt^{old} and Δt^{new} are the old and new time step values,

respectively. μ_1 and μ_2 are the constant coefficients and their typical ranges are from 1.1 to 1.5 and 0.3 to 0.9, respectively.

Equation (9) shows that if the number of iterations is small, the time step can be increased. In addition, if the number of iterations is more than maximum number of iterations, it shows that smaller time step is required.

In this study, the performance of the constant and automatic time stepping methods are evaluated for solving the h-based form of Richards equation. Also, the values of N_{max}, μ_1 and μ_2 are considered to be 30, 1.5 and 0.7, respectively.

D. Evaluation Criteria

Four criteria are considered for evaluation of the performance of numerical methods. These criteria are Root Mean Square Error (RMSE), mass balance conservation, number of iterations and execution time.

References [6] and [7] used RMSE for evaluation of numerical methods. Another evaluation method is the ability to conserve global mass over the domain of interest (mass balance conservation). Adequate conservation of global mass is necessary but not sufficient for acceptability of a numerical simulator [2]. Mass balance (MB) measurement for determination the ability of a scheme for mass conservation can be defined as (10) [2]:

$$MB(t) = \frac{\text{total additional mass in the domain}}{\text{total net flux int o the domain}} \qquad (10)$$

Where the additional mass is measured with respect to the initial mass in the system. For FD approximation with the first type boundary conditions, this is calculated as (11) [2].

$$MB(t^n) = \frac{\sum_{i=2}^{N-1}(\theta_i^n - \theta_i^0)\Delta z}{\sum_{j=0}^{n}\left\{-k_{N-1}^j\left[\dfrac{h_{N-1}^j - h_N^j}{\Delta z} + 1\right] + k_{3/2}^j\left[\dfrac{h_1^j - h_2^j}{\Delta z} + 1\right]\right\}\Delta t} \qquad (11)$$

Where $k_{N-1}^j = \dfrac{k_N^j + k_{N-1}^j}{2}$, $k_{3/2}^j = \dfrac{k_1^j + k_2^j}{2}$, N is the number of nodes, n is the number of time steps, h_N^j is the pressure head in the j-th time step and N-th node, θ_i^0 and θ_i^n are the initial and final values of moisture content in node i, respectively.

III. ILLUSTRATIVE EXAMPLES

Two different one-dimensional infiltration examples are investigated in this study.

In the first example, a constant pressure head into a vertical 40 cm column of soil is simulated [1]. A constant pressure head of -20.7 cm at the top of the column and a constant pressure head of -61.5 cm at the bottom are imposed as

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boundary conditions and a uniform pressure head of -61.5 cm is considered as the initial condition. The saturated and residual water content (θ_s and θ_r) are 0.287 and 0.075, respectively. The saturated hydraulic conductivity of the soil (k_s) is 0.00944 cm/s. The soil hydraulic property functions are [1]:

$$\theta(h) = \frac{\alpha(\theta_s - \theta_r)}{\alpha + |h|^{\beta}} + \theta_r \qquad (12)$$

$$K(h) = k_s \frac{A}{A + |h|^{\gamma}} \qquad (13)$$

Where $\alpha, \beta, A\ and\ \gamma$ are fitting parameters with the values of $1.611 \times 10^6, 3.96, 1.175 \times 10^6$ and 4.74, respectively.

Another constant head infiltration in a vertical column of very dry soil is considered as the second example. This problem was simulated by [2],[7]. The column has a length of 1 m. The initial condition was set as a constant pressure head of -10 m, while the upper and lower boundary values were set at -75 cm and -10 m, respectively. The saturated hydraulic conductivity is 0.00922 cm/s, and the saturated and residual water contents are 0.368 and 0.102, respectively. The Van Genuchten equations [8] are used for hydraulic properties of unsaturated soil.

$$\theta(h) = \frac{\theta_s - \theta_r}{\left[1 + (\alpha|h|)^n\right]^m} + \theta_r \qquad (13)$$

$$K(h) = k_s \frac{\left\{1 - (\alpha|h|)^{n-1}\left[1 + (\alpha|h|)^n\right]^{-m}\right\}^2}{\left[1 + (\alpha|h|)^n\right]^{m/2}} \qquad (14)$$

Which α, n and m are fitting parameters, with the values of 0.0335, 2.0 and 0.5, respectively.

The examples 1 and 2 are infiltration into the initially relatively wet and very dry soils, respectively.

IV. RESULTS AND DISCUSSIONS

In this study, all of the numerical codes have been written by MATLAB 6.0 software and executed on a Pentium-III, 1000 MHz system.

The example 1 was solved by different numerical schemes as 40 cm column with vertical grid spacing of $\Delta z = 1$ cm and elapsed time of 360 s.

The example 2 was solved by different numerical schemes as 1 m column of soil with vertical grid spacing of $\Delta z = 2.5$ cm and elapsed time of 86400 s. Numerical solutions of two examples with very dense grid spacing were considered as the exact solutions for determination of RMSE of numerical schemes.

Tables III and IV show the results of numerical solution of

examples 1 and 2 by fully implicit scheme, respectively. The results show poor mass balance when the tangent method is used for approximation of moisture capacity. Reference [2] reported similar findings. The comparison between the tangent and SCS approximations of moisture capacity shows that SCS approximation can improve the mass balance and RMSE values, however its execution time is more than tangent method. Similar findings have been reported by [3]. Table IV shows that SCS approximation has better convergence than tangent approximation. Fig. 1 shows the numerical solutions of two examples using SCS approximation. The results of numerical solution using different time stepping and convergence criteria show that automatic time stepping with δ_θ as convergence criterion can generally lead to better numerical results.

According to the numerical results, it is easy to judge that fully implicit scheme with SCS approximation, automatic time stepping and δ_θ as convergence criterion can achieve to reliable results.

Numerical solutions of h-based Richards equation by C-N scheme with constant time stepping often did not converge for the Δz and Δt values, presented in Tables III and IV. For instance, in the examples 1 (Δz=1.0) and 2 (Δz=2.5), the C-N scheme with tangent approximation and δa as convergence criterion can converges when the Δt is less than 1.6 and 5 s, respectively. However, C-N scheme with automatic time stepping method showed better convergence than constant time stepping method.

The results of numerical solution by Runge-Kutta scheme showed worse results than C-N scheme.

These results demonstrate that the fully implicit scheme is better and more reliable than C-N and Runge-Kutta schemes.

V. CONCLUSION

Among the different numerical schemes (Fully implicit, Crank-Nicolson and Runge-Kutta schemes), the fully implicit scheme is better than other schemes for numerical solution of h-based Richards equation. In addition, Utilizing of SCS approximation of moisture capacity, automatic time stepping and δ_θ as convergence criterion in the fully implicit scheme can improve the performance of the scheme.

C-N scheme is better than Runge-Kutta for solution of h-based Richards equation.

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REFERENCES

[1] R. Haverkamp, M. Vauclin, J. Touma, P. J. Wierenga, and G. Vachaud, "A comparison of numerical simulation models for one-dimensional infiltration," *Soil Soc. Am. J.,* vol. 41, pp. 285−293, 1977.

[2] M. A. Celia, B. T. Bouloutas, and R. L. Zarba, "A general mass conservative solution for the unsaturated flow equation," *Water Resour. Res.,* vol. 26, pp. 1483–1496, 1990.

[3] K. Rathfelder, and L. M. Abriola, "Mass conservative numerical solutions of the head based Richards equation," *Water Resour. Res.*, vol. 30, pp. 2579–2586, 1994.

[4] P. S. Huyakorn, and T. D. Wadsworth, "FLAMINCO: a three dimensional finite element code for analyzing water flow and solute transport in saturated-saturated porous media," Geo. Trans. Inc., Herndon,VA, 1985.

[5] K. Huang, B. P. Mohanty, and M. T. Van Genuchten, "A new convergence criterion for the modified Picard iteration method to solve the variably saturated flow equation," *Journal of Hydrology*, vol. 78, pp. 69–91, 1996.

[6] S. O. Magnuson, R. G. Baca, and A. J. Sondrup, "Independent verification and benchmark testing of the PORFLO-3 computer code," version 1.0, Idaho Natl. Lab., Idaho, Rep. EGG-BG-9175, 1990.

[7] A. I. El-Kadi, and G. Ling, "The Curant and Peclet number criteria for the numerical solution of Richards equation," *Water Resour. Res.*, vol. 29, pp. 3485–3494, 1994.

[8] M. Th. Van Genuchten, "A closed form equation for predicting the hydraulic conductivity of saturated soils," *Soil Soc. Am. J.*, vol. 44, pp. 892–898, 1980.

TABLE III
RESULTS OF NUMERICAL SOLUTION OF EXAMPLE 1 USING FULLY IMPLICIT SCHEME (ELAPSED TIME=360 S AND ΔZ=1 CM), C AND A ARE CONSTANT AND AUTOMATIC TIME STEPPING METHODS

Time Stepping Method	Convergence criterion	MB Δt			RMSE Δt			Iteration Number Δt			Time of CPU (s) Δt		
		10	30	120	10	30	120	10	30	120	10	30	120
Tangent C	δa	0.92	0.87	0.81	0.06	0.27	0.53	173	104	54	0.99	0.61	0.27
A	δ_θ	0.94	0.91	0.87	0.07	0.10	0.51	330	205	122	1.7	1.04	0.66
	δa & δr	0.89	0.87	0.85	0.17	0.28	0.21	63	55	42	0.33	0.28	0.22
SCS C	δa	1	1	1	0.09	0.15	0.37	175	105	58	1.1	0.7	0.4

TABLE IV
RESULTS OF NUMERICAL SOLUTION OF EXAMPLE 2 USING FULLY IMPLICIT SCHEME (ELAPSED TIME=86400 S AND ΔZ=1 CM)

| Time Stepping Method	Convergence criterion	MB Δt				RMSE Δt				Iteration Number Δt				Time of CPU (s) Δt			
		20	144	720	3600	20	144	720	3600	20	144	720	3600	20	144	720	3600
Tangent C	δa	0.98	-	0.83	0.6	15.8	-	7.7	56.0	9135	-	856	579	41.9	-	3.9	2.7
A	δ_θ	0.95	0.95	0.95	0.95	3.9	4.0	3.5	3.9	819	824	837	822	3.84	3.79	3.9	3.8
	δa & δr	0.87	0.88	0.8	0.68	29.9	23.3	28.5	33.9	322	327	273	244	1.48	1.54	1.27	1.15
SCS C	δa	1	1	1	1	16.9	16.7	16.7	21.2	9709	1977	757	491	54.8	11.5	4.3	2.8
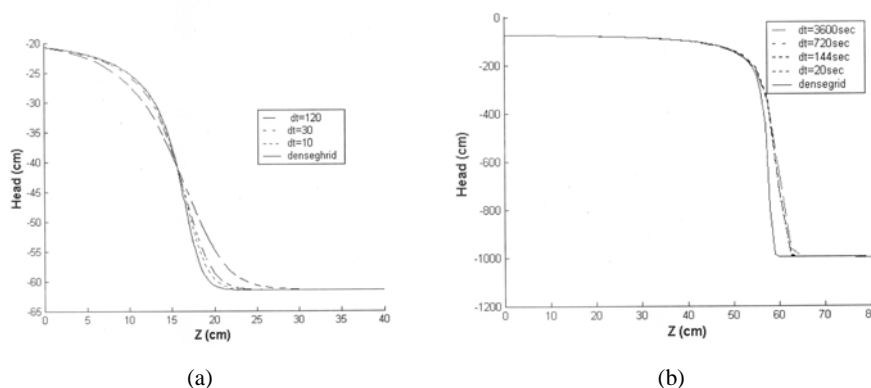
Fig. 1 Results of numerical solutions by fully implicit scheme with SCS approximation, a: example 1 (Elapsed time=360 s and ΔZ=1 cm), b: example 2 (Elapsed time=86400 s and ΔZ=2.5 cm)