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A CRITICAL APPRAISAL OF NUMERICAL MODELING OF WATER FLOW DYNAMICS IN UNSATURATED HOMOGENEOUS POROUS MEDIUM

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ABSTRACT

The assessment different forms of one-dimensional Richards' equation for the dynamics of water flow through unsaturated homogeneous porous media was reviewed comprehensively and it was found that the mixed (and h) based form of the Richards' equation maintained the mass-conservative properties in comparison with the -based and h-based equations. The review of the numerical methods showed that the fully implicit schemes for the finite difference discretization of the mixed-based mathematical formulation gave comparatively better performance. An appraisal of the averaging methods for hydraulic functions in terms of unsaturated hydraulic conductivity was made and it was observed that the geometric mean gave comparatively better results. The performance of the numerical scheme was also reviewed and it was found that a non-linear convergence criterion improved the computational efficiency in comparison to standard convergence criterion.

Keywords- *Flow dynamics, unsaturated media, numerical methods, convergence criteria.*

I. INTRODUCTION

The water flow dynamics in the unsaturated porous medium is an important phenomenon and is used in various hydrological and solute transport problems. It is simulated by using 3-D Richards' equation (1931) with appropriate initial and boundary condition and is expressed as:

$$\frac{\partial\theta\,(h)}{\partial t} = \nabla.\,[K\,(h)\nabla H] \qquad (1)$$

Upon reducing Eq. (1) to 1-D (vertical direction) equation, the different standard forms of Richards' equations (2a, 2b and 2c) are obtained by embedding the Darcy's law ($q = -K\,(h)\,\partial H/\,\partial z$; q , H (= h + z) , h and z are the flux density [L/T], total hydraulic head [L], soil water suction head [L] and the gravitational head [L], respectively) into the continuity equation (conservation of mass i.e. $\partial\theta\,(h)/\,\partial t = -\partial q/\,\partial z$; θ (h) and t are the soil water content $[L^3/L^3]$ as a function of h and the elapsed time [T], respectively). For the capillary rise phenomenon in the unsaturated media from the fixed water table, both these hydraulic heads i.e. h and z are acting in the opposite directions and hence H = h − z. These three standard forms i.e. the mixed (θ and h) -based, soil water suction head-based (h-based) and the soil water content- based (θ-based), respectively can be written as:

$$\frac{\partial\theta\,(h)}{\partial t} = \frac{\partial}{\partial z}\left[K\,(h)\,\frac{\partial h}{\partial z}\right] - \frac{\partial K\,(h)}{\partial z} \qquad (2a)$$

$$C\,(h)\,\frac{\partial h}{\partial t} = \frac{\partial}{\partial z}\left[K\,(h)\,\frac{\partial h}{\partial z}\right] - \frac{\partial K\,(h)}{\partial z} \qquad (2b)$$

$$\frac{\partial\theta\,(h)}{\partial t} = \frac{\partial}{\partial z}\left[D\,(\theta\,(h))\,\frac{\partial\theta\,(h)}{\partial z}\right] - \frac{\partial K\,(\theta(h))}{\partial z} \qquad (2c)$$

Where z is the vertical distance measured positive upward for the capillary rise from the fixed water table [L]; K (h) or K $(\theta\,(h))$ is the unsaturated hydraulic conductivity of the medium [L/T] ; C (h) (= dθ/dh i.e. first derivative of the soil water retention function) is the specific (differential) water capacity $[L^{-1}]$ and D (θ (h)) (= K $(\theta\,(h))$/ C$(\theta\,(h))$) is the unsaturated water diffusivity of the porous medium $[L^2/T]$, respectively. In these formulations the soil water suction head h was taken as positive [L] and while defining the total hydraulic head H soil water suction head, the osmotic potential caused by the salt concentration was assumed to be negligible in comparison with the sum of the soil water suction and the gravitational heads. The soil water content (θ) and the soil water suction head (h) have been taken as uniquely related which allowed for conversion of one form into the other i.e. $\partial\theta/\partial t$ can be taken as $(d\theta/dh)$ $(\partial h/\partial t)$ and $\partial h/\partial z$ as $(dh/d\theta)$ $(\partial\theta/\partial z)$. The thermal effects have been neglected and the fluid density was assumed unaffected by the solute concentrations. Despite these limitations and assumptions, Hoffmann (2003) reported that the Richards's equation still remains the most widely used equation for the flow of water through the unsaturated soil medium.

These different forms of the Richards' equation contain two terms on the right hand side, whereas the first term expresses the contribution to the unsaturated flow by the soil water suction head gradient while the second term expresses the contribution by the gravitational head, respectively. These second order parabolic partial differential equations are highly non-linear as the non-linearity is caused by the variable hydraulic coefficients of the hydraulic conductivity, soil water capacity and the water diffusivity which are the functions of the dependent variables i.e. θ or h which in turn are the functions of the space in the flow domain at different times of the capillary rise phenomenon .Van Genuchten (1980) reported that the small changes in the soil water suction head (h) can change the hydraulic functions of conductivity several orders of magnitude and as such the non-linearity is high. Also the soil water content (θ) as a function of the soil water suction head is also highly non-linear as the degree of saturation can change dramatically over a small range of soil water suction head. Due to the importance for their applications to the practical problems, many investigators devoted their efforts for the proper assessment of different forms of Richards' equation. Vasconcellos and Amorim (2001) reported that the mixed-based formulation of the Richards' equation provides the most direct mathematical expression of the physics of the unsaturated flow and thus is the most fundamental formulation. Earlier, Celia et al. (1990) and Huang et al. (1996) also reported that the mixed-based formulation of the Richards' equation maintained the mass conservative properties. it was observed that most of the unsaturated flow simulations either used the h-based formulation or the θ-based formulation prior to the mass-conservative mixed-based numerical simulation of the unsaturated flow through the porous medium as proposed by Celia et al. (1990).

II. FINITE DIFFERENCE NUMERICAL SCHEMES

For the numerical solution of the Richards' equation, numerical methods are based on subdividing the flow region into finite segments bounded and represented by a series of nodal points at which the solution is obtained. For the finite difference approximation, different discretization schemes such as explicit, implicit Crank-Nicolson (second order implicit method in time) and fully implicit schemes are employed. In the explicit scheme, linearization by explicit time discretization using forward Euler method along with space discretization is used resulting into a series of linearized independent algebraic equations which are solved directly at each time level and thus it is computationally simple as far as the non-linearity in the original equation poses no difficulty in the discreet algebraic equations but in order to attain a reasonable accuracy, the space step must be kept small and to get a stable solution the time step has also to be kept small as compared with the space step. Thus the explicit finite difference scheme is not unconditionally stable. The implicit Crank-Nicolson is combination of the forward Euler method and the backward Euler method for time discretization and is unconditionally stable. The fully implicit method in which backward Euler scheme for time discretization is used for solution of mixed-based form results in the non-linear algebraic equations and these simultaneous non-linear algebraic equations are linearized by iterative methods resulting in the linear algebraic equations involving tridiagonal coefficient matrix with zero elements outside the diagonal. These linear algebraic equations after discretization, linearization and simplification are solved for unknown values of θ or h as a function of space in the flow domain at different times after incorporating appropriate initial condition and the boundary conditions either in the form of Dirichlet condition (prescribing the variable) or the Neumann condition (prescribing the derivative of the variable and thus specifying the flux) For a given grid point at a given time, the values of the hydraulic coefficients K (h) or K (θ (h)), C (h) or D (θ (h)) can be expressed in the form of constitutive relationship alongwith $\theta - h$ relation.

III. NUMERICAL SOLUTIONS OF RICHARDS' EQUATION

Because of the non-linearity of the hydraulic functions in terms of the variable coefficient and the θ (h) function, the analytical solutions are not possible for these equations except for some special cases. However, these were solved analytically by Srivastava and Yeh (1991) Arampatzis et al. (2001) and Menziani et al. (2007) and some others which are valid for simple initial and boundary conditions along with simplification of hydraulic functions. Assouline (2013) also reported that the analytical solutions can only be derived for the simplified flow cases under number of restrictive assumptions and are rather scarce. Therefore, these non-linear partial differential mathematical formulations of different forms were solved with approximations employing space discretization methods: finite difference method (Celia et al.,1990; Tocci et al., 1997 and Miller et al., 1998) and the finite element method (Celia et al.,1990 ; Forsyth and Pruess ,1995 ; Simunek et al., 1998; Bergamaschi and Putti, 1999; Kavestki et al., 2001) and finite volume method (Forsyth and Pruess, 1995 and McBride et al., 2006). Van Genuchten (1982), Pan et al. (1996) and Islam and Hasan (2014) reported that for one-dimensional unsaturated flow in the porous media, the finite difference is comparatively more advantages because it does not need mass lumping to prevent oscillations as in the finite element method as the standard Galerkin approach produces oscillations in the solution. For time discretization (time-marching stepping) Kavetski et al. (2002) reported that the time discretization by implicit backward Euler approximation has been employed by many investigators which is first order accurate but very stable. The algebraic system of highly non-linear equations after temporal and spatial discretizations are solved in each time step by linearizing the non-linear function by the use of the iterative solvers such as the Picard (also known as the fixed-point iteration, successive substitution or the non-linear Richardson iteration) or the Newton iterations which are the most common non-linear iterative solvers (Paniconi and Putti, 1994). Celia et al. (1990) proposed the modified Picard method which performed much better than the classical Picard method. Lehman and Ackerer (1998) reported that the Picard iterative solver is comparatively more prevalent due its simplicity and generally acceptable performance. Szymkiewicz (2004) also reported that the Picard method requires less computational efforts and performed well for the unsaturated flow solutions without sink or source term.

IV. PERFORMANCE OF DIFFERENT FORMS OF RICHARDS' EQUATION

Hills et al. (1989) reported that the discrete approximation of the θ-based form of the Richards' equation can be formulated in the mass-conservative form and can conserve mass within the computational domain regardless of the space and time steps using the finite difference implicit scheme but the limitation of this formulation is that it cannot be used for describing the flow in the saturated media as in this media soil water content does not change with time and also in the layered soils as the soil water content and consequently the water diffusivity function exhibit the discontinuity at the interface between the adjacent layers having different hydraulic properties. So, this form can only be applied for the flow in the homogeneous porous media. Celia et al. (1990) also reported that the θ −based formulation of flow cannot be applied to the fully saturated flow condition as for the saturated flow, the time derivative of the soil water content vanishes but not the space derivative of the positive total water head and also cannot be applied for non-homogeneous soils as the discontinuous θ- profiles are produced at the interface in such stratified soils. Islam (2015) reported that the θ-based algorithm may also suffer from mass balance errors at the boundaries even when this formulation can accurately conserve the mass in the interior of the flow domain. So the mixed-form of unsaturated flow allows a mass conservative solution can also be applied to the saturated as well as stratified soils. However, the h-based form can also be applied to both the saturated and the unsaturated flows and for the layered soils, but Hills et al. (1989) and Celia et al. (1990) reported the high global mass balance error (the mass balance is measured by the ratio of the total additional mass in the domain to the total net flux into the domain; and the additional mass balance is measured with respect to the initial mass in the system) in the numerical solution for the domain of interest and thus showed poor mass conservative properties with unacceptably large mass balance errors to the extent of greater than 10 percent for any iteration method.

Celia et al. (1990) further reported that the poor mass balance resides in the time derivative of the soil water suction head (h) when the h-based formulation is used, as the finite difference approximation based on the h-based and mixed-based forms are different in the sense that the mixed-based finite difference approximation contains the mass balance term as an additional term in comparison with the h-based finite difference approximation. This additional term was obtained in the finite difference of approximation of the mixed-based form by linearizing the non-linear soil water contain function in the time derivative term with the truncated Taylor series expansion retaining only the terms upto the first order. This linearization and with the fully implicit (backward Euler) time approximation applied to the mixed-based formulation revealed that the mixed- based form possesses better conservative property than the h-based formulation (Celia et al., 1990) as reported above. They further highlighted the fact that the proper treatment of the time derivative of the mixed-based formulation is critical in the numerical solution of the unsaturated flow in the porous media. In this regard they explained that while $\partial\theta/\partial t$ in the mixed-based form and its chain-rule splitting into C(h) ($\partial h/\partial t$) for derivation of h-based form from the θ-based form are mathematically equivalent in the continuous partial differential equation of the unsaturated flow but their discrete analogs are not equivalent as the inequality in the discrete form is aggravated by the highly non-linear nature of the specific water capacity term C(h) leading to the significant mass balance error in the h-based formulation .From this, it can be seen that the change in mass in the system is estimated using the discrete values of $\partial\theta/\partial t$ and not by the product of C(h) and ($\partial h/\partial t$) in the discrete form . So in conclusion it can be stated that the chain-rule splitting of the time derivative of the soil water content into two components is equivalent in the continuous domain but in the discretized domain it is not the same leading to non-conservative of mass when h-based form is applied to the unsaturated flow problems, while the mixed-based form does not separate the continuous form of the Richards' equation but instead expands the non-linear function θ(h) using Taylor series about the pth iterate of θ to approximate $h^{j+1,p+1}$; j and p being time and iteration levels. Thus the use of the mixed-based formulation led to the significant improvement in the performance of the numerical solution as it combines benefits inherent in both the θ-based and h-based forms while circumventing major problems associated with each.

Ray and Mohanty (1992) also used different finite difference schemes for the solution of the h-based and the mixed-based formulations and showed that the mixed-based formulation gave better results than the h-based formulation. Kumar (1998) simulated the transient unsaturated flow through the homogeneous and isotropic soil using the h-based form of the Richards' equation instead of mass-conservative mixed-based with finite difference approximation in the form of explicit, Crank-Nicolson and fully implicit discretization schemes with the geometric mean for the internodal unsaturated hydraulic conductivities and reported that the simulated water content profiles for the infiltration process in the homogeneous semi-infinite soil column using the implicit finite difference approximation were in better agreement with the quasi-analytical solution of the Richards' equation by Philip (1957) as analytically derived in the form of power series of time elapsed subject to the condition of a constant head at the soil surface. He did not evaluate the mass balance error. Shahraiyni and Ashtiani (2012) made comprehensive evaluation of the different finite difference schemes i.e. the fully implicit, Crank-Nicolson and Runge-Kutta (one step-two stages) for the solution of the h-based formulation with Picard iteration method and the mixed-form of the Richards' equation with the modified Picard method as proposed by Celia et al. (1990) for the prediction of the water infiltration into the soil. The results of the numerical simulation showed that the fully implicit scheme for the finite difference discretization of the mixed-form formulation gave better performance in terms of the mass balance and the convergence than the h-based form.

Vasconcellos and Amorim (2001) used the finite difference approximation obtained by the backward Euler method for the temporal discretization coupled with the fully implicit modified Picard iterative procedure for all the three different formulations of the one-dimensional non-linear Richards' equation for simulation of the infiltration process in the homogeneous soil. In the mixed-based form instead of directly solving the discretized formulation, for the soil water content profiles they incorporated the expansion of the soil water content at the i space level ($\theta_i^{j+1,p+1}$) at the next time (j+1) and the iteration (p+1) levels using the truncated Taylor series with respect to the soil water suction head (h) about the expansion point h at the next time step (j+1) and at the previous iteration level (p) simulating the soil water suction head profiles. Based on their analysis, they reported that the h-based form generated poor results characterized by the large mass-balance errors while the solution based on the mixed-form of the Richard's equation is the most mass-conservative solution. Ross (2003) introduced a non-iterative solution for the Richards' equation using the soil hydraulic properties as proposed by Brooks-Corey (1964) and used a space-time discretization scheme in order to derive a tridiagonal set of linear equations which were solved non-iteratively. Vardo et al. (2006) later conducted a thorough assessment of the method proposed by Ross (2003) and concluded that the model provided robust and accurate solution as compared with the analytical solution of Basha (1999).

The above stated investigations were conducted for the infiltration process but Htel et al. (2013) simulated the capillary rise of the water in the porous media using the h-based Richards' equation instead of using mass-conservative mixed-based form by the finite difference discretization with the implicit method and using the arithmetic mean for the evaluation of the internodal unsaturated hydraulic conductivities at the mid-point between the adjacent nodes solving a system of simultaneous linear algebraic equations with a tridiagonal coefficient matrix with zero elements outside the diagonal for the unknown values of h (z, t).

V. EVALUATION OF AVERAGING METHODS FOR HYDRAULIC FUNCTIONS:

As stated earlier, the variable hydraulic functions of the conductivity, water diffusivity and water capacity are non-linear in nature and are needed to be approximated by linearization. One of the important factor influencing the accuracy of the numerical solution of the one-dimensional unsaturated flow equation is the averaging method applied to compute these hydraulic functions between two adjacent nodes of the computational domain of the homogenous soil. Also in order to compute the corresponding water flux, it is necessary to estimate the weighted values of these parameters between the adjacent nodes as a function of known values of soil water suction heads. For the approximation of the internodal (weighted) hydraulic conductivity ($K(h_{i\pm1/2})$), different weighting techniques in terms of the arithmetic mean (($K(h_i)+K(h_{i\pm1})$)/2), harmonic mean ((2 $K(h_i)K(h_{i\pm1})$)/($K(h_i)+K(h_{i\pm1})$)), the geometric mean ($\sqrt{K(h_i)K(h_{i\pm1})}$) and upstream mean for modeling one-dimensional water flow in homogeneous unsaturated soil were proposed and tested by Haverkamp and Vauclin (1979) for studying their influence on the accuracy of the finite difference solution and observed that the geometric mean simulated well their experimental observations. Also other propositions for approximating the internodal hydraulic function can be found in Haverkamp et al. (1977) and Miller et al. (1998). Miller et al. (1998) reported that the internodal conductivities can also be estimated by the integration of K(h) in the interval (h_i, $h_{i\pm1}$). Hornung and Messing (1983) also reported that the geometric mean for evaluation of the internodal hydraulic conductivity gave better results. Schnabel and Richie (1984) also recommend the use of the geometric mean for the estimation of the weighted hydraulic conductivity. Based on review of many investigation, Szymkiewicz and Helmig (2010) reported that the accuracy of the numerical solution is sensitive to the choice of the approximating method for weighted hydraulic conductivities especially on coarser grids. On the other hand Dam and Feddes (2000) reported that the influence of the method of approximation becomes insignificant for small values of space steps. However, while evaluating the numerical solutions of the h-based and mixed-based formulations of the Richards' equation, Celia et al. (1990) used the arithmetic mean for the estimation of the internodal hydraulic conductivities. Warrick (1991) used a more sophisticated approach for averaging the hydraulic conductivity based on the local solution of the steady state flow between the adjacent nodes (Darcian means) by which average conductivity is chosen in such a manner that the resulting flux is equal to the flux obtained from the solution of the steady state flow equation between two adjacent nodes. However, Szymkiewicz and Helmig (2010) reported that this Darcian means a method is unsuitable for practical applications. Another method for approximating the internodal hydraulic conductivity was proposed by Zaidel and Russo (1992) in which the hydraulic conductivity is approximated by taking first the arithmetic mean of the effective saturation at the adjacent space nodes and then estimating hydraulic conductivity at that resulting effective saturation. Vasconcellos and Amorim (2001) used arithmetical mean, geometric mean and the harmonic mean in estimating the interblock unsaturated hydraulic conductivity between the neighbor points of the mesh. The weighted values of the soil water diffusivity can also be approximated in the same manner as done for weighted value of the hydraulic conductivity. For approximation of the non-linear soil water capacity, either the tangent approximation or the standard chord slope (SCS) approximation can be performed as reported by Shahraiyni and Ashtiani (2012). Rathfelder and Abriola (1994) have shown that the SCS approximation to the specific water capacity C(h) in the form $\partial\theta/\partial h \approx ((\theta^{j+1}-\theta^{j})/(h^{j+1}-h^{j})$; j being the time level) improved the mass balance of the numerical scheme for the h-based Richards' equation in comparison to the analytical derivative of θ(h) as tangent approximation (C(h) = dθ/dh). However, Shahraiyni and Ashtiani (2012) reported that the numerical scheme of the mixed-based form with SCS approximation had no significant effect on the solution results of the mixed-form but showed better convergence than the tangent approximation. The hydraulic function of non-linear soil water capacity C(h) as tangent approximation in the time-stepping term can either be evaluated at the current time level or at the previous time level.

VI. CONVERGENCE CRITERIA FOR NUMERICAL SCHEMES

For the performance of the numerical scheme, the criterion of convergence is important aspect as the numerical solution should approach to the exact solution of the governing partial differential equation as the grid size tends to zero. Different criteria have been used by the investigators. Celia et al. (1990) applied the standard convergence criterion to judge the convergence status of the mixed-form algorithm wherein the iterative process continuous until the difference between the calculated values of the soil water suction head between two successive iteration levels ($\delta^{p}=h^{j+1,p+1}-h^{j+1,p}$) becomes less than a preset tolerance level. Huang et al. (1996) reported that this standard criterion is valid for the h-based algorithm but may also be used for the mixed-form algorithm of Celia et al. (1990) as this scheme actually solves for the soil water suction head $h^{j+1,p+1}$ as for the h-based formulation. They further improved the computational efficiency of the modified Picard method of the mixed-form algorithm of Celia et al. (1990) by accelerating the rate of convergence through a non-linear convergence criterion based on the product of the specific water capacity ($C^{j+1,p}$) and the absolute error δ^{p} as derived using the Taylor series expansion of the soil water content at the next time and iteration levels and also further reported that the standard convergence criterion also produced the perfect mass balance.

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