IJE TRANSACTIONS A: Basics Vol. 28, No. 4, (April 2015), 490-498

International Journal of Engineering

Journal Homepage: www.ije.ir

Selection of Intermodal Conductivity Averaging Scheme for Unsaturated Flow in Homogeneous Media

M. Sayful Islam*

Department of Mathematics, Shahjalal University of Science & Technology, Sylhet, Bangladesh

PAPER INFO

Paper history:
Received 08 October 2014
Received in revised form 29 December2014
Accepted 29 January 2015

Keywords:
Richards' Equation
Variably Saturated Flow
Internodal Conductivity
Infiltration
Finite Difference

ABSTRACT

The nonlinear solvers in numerical solution of water flow in variably saturated soils are prone to convergence difficulties. Many aspects can give rise to such difficulties, like very dry initial conditions, which causes a steep pressure gradient and great variation of hydraulic conductivity occurs across the wetting front during the infiltration of water. So, the averaging method applied to compute hydraulic conductivity between two adjacent nodes of the computational grid is one of the most important issues influencing the accuracy of the numerical solution of one-dimensional unsaturated flow equation i.e., Richards' equation. A number of averaging schemes such as arithmetic, geometric, harmonic and arithmetic mean saturation have been proposed in the literature for homogeneous soil. The resulting numerical schemes are evaluated in terms of accuracy and computational time. It can be seen that the averaging scheme in the framework of arithmetic approaches favorably to other methods for a range of test cases.

***doi**: 10.5829/idosi.ije.2015.28.04a.01*

1. INTRODUCTION

Water flow in partially saturated porous medium is commonly described with a nonlinear partial differential equation, known as the Richards' equation and closed by constitutive relations to describe the relationship among fluid pressures, saturations, and relative permeabilities [1, 2]. Its one-dimensional form is often used in hydrological and agricultural engineering to predict changes of water content and fluxes in the soil profile, which in turn can be used as input in larger scale hydrological models or contaminant transport models. The same equation can be also used to simulate moisture transport in building materials or other industrial porous materials. Richards' equation is derived by combining Darcy's law with mass conservation equation in porous media. For the case of one-dimensional flow in an arbitrary spatial direction it can be written into one of the following forms:
Mixed, or coupled form of Richards' equation:

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}\left[K(\psi)\left(\frac{\partial \psi}{\partial z}+1\right)\right] \tag{1}$$

where ψ is the pressure head [L], θ(ψ) is the volumetric soil moisture content [$L^3\ L^{-3}$], K(ψ) is the nonnegative hydraulic conductivity [LT^{-1}], t is the time [T], and z is the vertical coordinate assumed positive upward [L].
Pressure-based, ψ-form of Richards' equation is:

$$c(\psi)\frac{\partial \psi}{\partial t} = \frac{\partial}{\partial z}\left[K(\psi)\left(\frac{\partial \psi}{\partial z}+1\right)\right] \tag{2}$$

where $c(\psi) = \frac{d\theta}{d\psi}$ is the moisture capacity [L^{-1}].
Moisture-based, θ-form of Richards' equation is:

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}\left[D(\theta)\frac{\partial \psi}{\partial z}\right] + \frac{\partial K}{\partial z} \tag{3}$$

where $D = \frac{K}{c(\psi)} = K\frac{d\psi}{d\theta}$ is the soil water unsaturated diffusivity [$L^2\ T^{-1}$]. The ψ-based formulation is considered to be more useful for practical problems involving flow in layered or spatially homogeneous soils, as well as for variably saturated flow problems. Unfortunately, simulation of infiltration in dry and/or high nonlinear soils using ψ-based formulation often

*Corresponding Author's Email: sislam_25@yahoo.com (M. Sayful Islam)

Please cite this article as: M. Sayful Islam, Selection of Intermodal Conductivity Averaging Scheme for Unsaturated Flow in Homogeneous Media, International Journal of Engineering (IJE), TRANSACTIONS A: Basics Vol. 28, No. 4, (April 2015), 490-498

faces difficulties in conserving mass. Water-content-based schemes 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 [3]. 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, and also is not easy to simulate. 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 systems. Whereas in the mixed form the mass is perfectly conserved, improving the accuracy of the results without requiring any additional computational effort. However, conservation of mass is shown to be insufficient to guarantee good numerical solutions.

The numerical simulators have been paid the most attention to overcoming the nonlinearity of flow and mass transport problems and reducing numerical dispersion and artificial oscillations in modeling flow in variably saturated porous media. In comparison, little efforts have been directed to elimination or reduction of mass balance error. Mass balance is defined as the ratio of the total masses of fluid added to the domain to the total net flux into the domain [4]. An accurate numerical simulator should conserve mass over entire spatiotemporal domain. A standard approach to reduce mass balance error in a highly nonlinear equation or a set of coupled nonlinear equations is using small time steps and iterative procedures, which in turn makes the solution very time consuming. Global mass balance errors may not be totally eliminated for severe nonlinear problems even when very small time step sizes are used [5]. To obtain the numerical solution of variably saturated one-dimensional flow problems, finite-difference approximations have been widely used in several studies [6- 10]. Fewer researchers have used finite differences to solve variable saturated flow problems in higher dimensions [11- 13].

Most of the existing two-dimensional finite-difference solutions to variably saturated flow problems are not robust because they incur numerical instabilities and convergence difficulties [11, 14, 15]. These problems arise primarily from inefficiencies of the line successive over-relaxation and alternating directional implicit schemes used in solving the two-dimensional, nonlinear equations. The most successful and efficient example of a finite-difference solution to two-dimensional, variably saturated flow problems has been established [12]. A competitive numerical procedure to solve infiltration problems in dry soils is developed which is not account for the effects of specific storage, and consequently it cannot be used to model accurately a wide variety of variably saturated flow problems, including many transient drainage and seepage face phenomena in large domains [12].

Low order finite difference method (FDM) or finite element method (FEM) [4, 16- 19], mixed-hybrid FEM [20] and discontinuous Galerkin FEM [21] schemes are usually performed to spatial discretization of Equation (1). To avoid oscillations FEM discretization mass-lumping must be applied [4]; standard low-order FEM leads to essentially the same discrete equations as FDM. In order to compute the corresponding water flux, it is necessary to estimate the average value of the hydraulic conductivity between adjacent nodes for each case. The most popular averaging schemes include arithmetic, geometric, upstream and integrated means. This is shown by numerous studies [20, 22-29] the accuracy of the numerical solution is sensitive to the choice of the averaging method, especially on coarser grids. Using adaptive grid refinement [21, 30, 31] or by using a transformed variable instead of the water potential head in Equation (1) [32, 33], however such approaches imply additional algorithmic complexity; the error can thus be significantly reduced. Hence, there is still some interest in developing improved averaging schemes that can be used in the framework of standard fixed-grid numerical algorithms.

A significant improvement in accuracy is obtained by using Darcian means approach [34]. The average conductivity is chosen in such a manner that the resulting flux is equal to the flux obtained from the solution of steady state flow equation between the two nodes according to this method. As a result the internodal conductivity depends on the distance between the nodes, except for the case of horizontal flow. Predominantly $K(\psi)$ that functions the computation of "true" Darcian means requires numerical solution of steady state problem. This makes the method unsuitable for practical application. Although it can be used, only as a starting point for the development of approximate averaging formulas, which can be more readily implemented in practice [22, 23, 28, 35, 36]. The effect of variable coefficient of permeability for a confined seepage problem under non-homogeneous and anisotropic conditions is successfully examined using least square finite element formulation [37].

The objective of this work is to develop and present a computationally simple and efficient finite-difference algorithm that can solve one-dimensional variably saturated flow problems using standard solution approaches and to evaluate the accuracy, efficiency and robustness of four selected averaging schemes for a range of porous media conditions.

2. SPATIAL DISCRETIZATION

In order to separate between numerical errors associated with the water content or capillary pressure head distributions and the evaluation of the flux at the soil surface, we consider the problem of solving Equation (1) given the following initial and boundary conditions:

$$\psi(z,t=0)=\psi_0(z),\\ \psi(z=0,t>0)=\psi_1,\\ \psi(z=Z,t>0)=\psi_2 \tag{4}$$

where ψ_0 is the initial condition and ψ_1 and ψ_2 are the given prescribed values of ψ and Z is the vertical extent of the flow domain.

A finite-difference approximation of Equation (1) on uniform grid spacing is assumed which transforms this partial nonlinear differential equation into the following set of nonlinear algebraic equation [38]:

$$[C(\psi_i)+S_sS_a(\psi_i)]\frac{d\psi_i}{dt}=\frac{1}{\Delta z^2}\left[K_{i-1/2}\psi_{i-1}-\left(K_{i-1/2}+K_{i+1/2}\right)\psi_i+K_{i-1/2}\psi_{i+1}\right]+\frac{1}{\Delta z}\left[K_{i+1/2}-K_{i-1/2}\right] \tag{5}$$

where i is a subscript denoting the grid point or cell $(0\le i\le N)$, $K_{i+1/2}$ is the interblock conductivity for calculating the capillary component of the water flux between cells $i+1$ and i depending on the unknown potentials ψ_{i-1}, ψ_i and ψ_{i+1}.

3.CONSTITUTIVE RELATIONSHIP

In order to solve Richards' equation, we have to specify the constitutive relations between the dependent variable pressure head and the nonlinear terms such as moisture content, moisture capacity and conductivity. The constitutive relations used in the work reported here is the van Genuchten [2] pressure-saturation relationship, which is given by:

$$S_e(\psi)=\frac{\theta(\psi)-\theta_r}{\theta_s-\theta_r} \tag{6}$$

where θ_r is the residual water content, θ_s is the water content at saturation, S_e is the effective saturation, α and n are the parameter depending on the pore size distribution and $m=1-\frac{1}{n}$. The specific moisture capacity $C(\psi)$ is defined as:

$$C(\psi)=(\theta_s-\theta_r)S_e'(\psi) \tag{7}$$

where $S_e'(\psi)$ is evaluated with the analytic differentiation of Equation (6).

The saturation-permeability relation is described using Mualem's [39] model for the relative permeability of the aqueous phase,

$$K(S_e)=K_sS_e^{\frac{1}{2}}\left[1-\left(1-S_e^{\frac{1}{m}}\right)^m\right]^2 \tag{8}$$

where K_s is the water-saturated hydraulic permeability and $S_e=S_e(\psi)$.

4. CONDUCTIVITY AVERAGING SCHEMES FOR HOMOGENEOUS SOILS

An imperative phase of this work is the approach used to estimate conductivities that vary in space as a function of ψ within the spatial discretization scheme. For soils with highly nonlinear properties, the accurate estimation of the interblock hydraulic conductivity is crucial. Various methods of estimation have been proposed in the finite-difference framework for calculating $K_{i+1/2}$ which differ considerably in their prediction of the flux and the water content distribution. In particular, these differences are most prominent near the wetting front where infiltration into dry soil is concerned [24, 32]. The most common approach for estimating the interblock conductivity $K_{i+1/2}$, when calculating the capillary component of the flux between numerical cells, is based on the arithmetic mean (AM) [24, 29, 34], i.e.

$$K_{i+1/2}=0.5(K_{i+1}+K_i) \tag{9}$$

This is simple and inexpensive to compute.

Another expression for estimating the interblock conductivity is that the geometric mean (GM) [24], i.e.,

$$K_{i+1/2}=\sqrt{K_{i+1}K_i} \tag{10}$$

The harmonic mean (HM) technique [24], for computing the interblock quantities can be expressed as:

$$K_{i+1/2}=\frac{2K_{i+1}K_i}{K_{i+1}+K_i} \tag{11}$$

The final approach considered for estimating $K_{i+1/2}$ is termed the arithmetic mean saturation (KMS) [29] and this method is easy to compute:

$$K_{i+1/2}=K\left[0.5\left(S_{e_{i+1}}+S_{e_i}\right)\right] \tag{12}$$

where S_e is the effective saturation. Some numerical studies published in the literature show that the methods listed above are not really universal, because their performance depends on the shape of the conductivity function, initial boundary conditions of the problem under consideration and grid size Δz [20, 22- 25, 28, 29]. A more accurate averaging technique is based on the assumption that the average conductivity should reproduce the steady-state flow rate between the two considered nodes, with the water potential values ψ_i and ψ_{i+1} taken as the boundary conditions.

5. RESULT AND DISCUSSION

Numerical experiments is performed to test the computer program and to investigate the behavior of different conductivity estimating techniques. Two tests are presented here involving the infiltration of water in homogeneous soil. An implicit ODE or DAE integrator, with a stiff solver MATLAB 'ode15s' which is based upon forms of the backward differentiation formulas is used. In order to assess the computational differences among the conductivity averaging schemes, first the model must be validated. This was achieved by independently testing the approaches against several benchmark problems. The benchmark results for the finite-difference have been previously discussed [38, 40]. For the matter of robustness and efficiency of the approaches, we study different features of ODE solver, such as, the number of successful steps, failed attempts, function evaluations, partial derivatives, LU decompositions, and solutions of linear systems. All of the numerical codes have been written by MATLAB 7.6.0 (2008a) software and executed on a Dell INSPIRON, 2.56 GHz system. Each test case was run with Relative Tolerance $RelTol = 1.0 \times 10^{-8}$ and Absolute Tolerance $AbsTol = 1.0 \times 10^{-10}$.

5. 1. Test Case 1 The first test case consists of infiltration into an unsaturated soil column for the van Genuchten model with the soil properties of $n = 2$, $\alpha = 3.35/m$, $\theta_r = 0.102$, $\theta_s = 0.368$, $K_s = 7.97\ m/day$. The initial conditions of a $0.3m$ high 1D soil column are initially dry with a pressure head $\psi_0(Z, 0) = -10\ m$. The boundary conditions are applied inhomogeneous Dirichlet with the top of the soil column $\psi_2(0.3, 0) = -0.75\ m$, and the bottom of the soil column $\psi_1(0, t) = -10\ m$. The initial conditions are not consistent with boundary conditions, and as such a steep gradient in the pressure head is setup. The spatial grid is uniform and as a spacing of *0.002 m*, the automatic time stepping is considered.

Van Genuchten hydraulic conductivity profile for different averaging techniques are presented in Figure 1. A comparison of the results exposed in this figure of snap shot (see Figure 2) shows the arithmetic mean conductivity averaging very little smears the steep wetting front more than other schemes.

Richards' equation has no analytic solution, which makes rigorous testing of the code more involved. The literature [38, 40] is a well documented example which provides qualitative agreement. Figures 3 and 4 are a comparison of solution profiles for uniform grids for pressure head and moisture content at different times for the arithmetic mean technique, respectively. Comparing the results obtained with this approaches shows excellent agreement [38, 40]; however, as the data is not provided it is impossible to evaluate quantitative agreement between the solutions.

In Figures 5 and 6 a comparison of the behavior of various conductivity averaging schemes of pressure head and moisture content profiles at the end of the simulation is shown. Graphical results indicate that the AM, GM, and KMS permeability estimation techniques are more robust than HM.

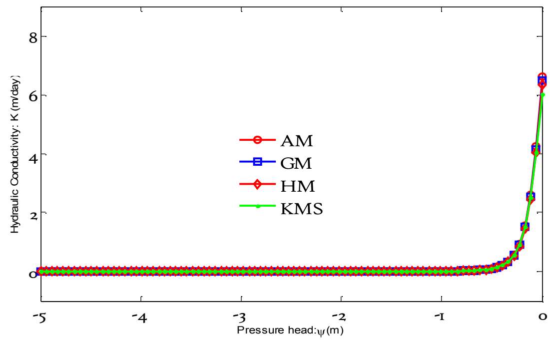

Figure 1. Hydraulic conductivity profiles for four averaging schemes.

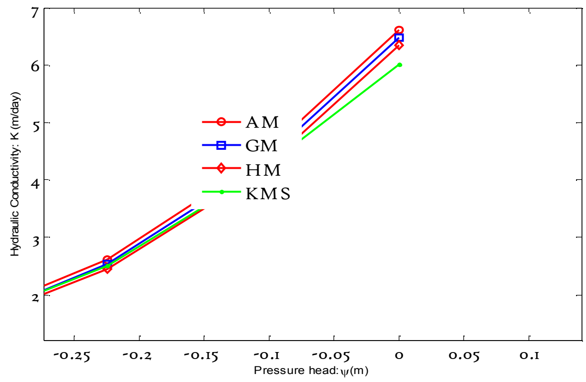

Figure 2. Snap shot of hydraulic conductivity profiles for four averaging schemes.

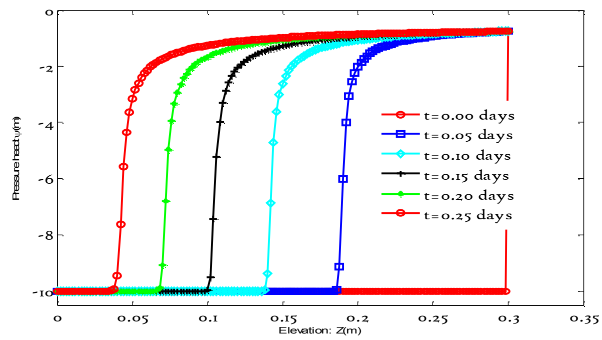

Figure 3. Pressure head profiles of AM averaging technique.

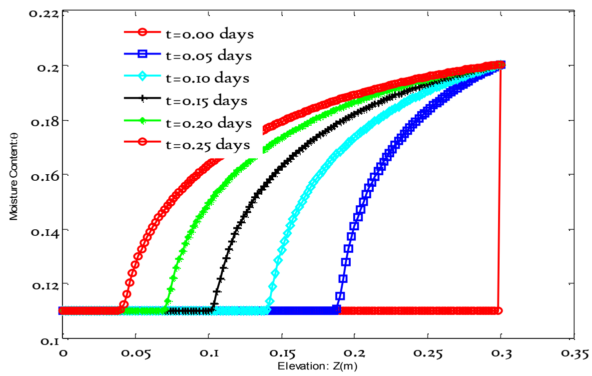

Figure 4. Water content profiles of AM averaging technique.

It is noted that numerical error is produced at the bottom of the soil column based on the harmonic mean averaging. Several points can be highlighted from the simulation such as the number of successful steps, the number of function evaluations, the number of Jacobian evaluations, the number of LU decomposition, and the total CPU time for each permeability estimation technique shown in Table 1. It can be seen that the computational performances produced by the various intermodal conductivity techniques are much closed except for harmonic mean technique.

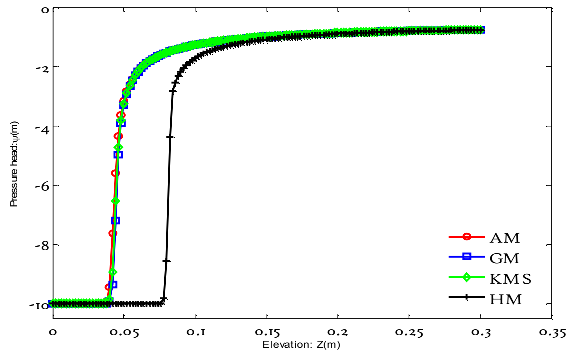

Figure 5. Pressure head profiles of AM, GM, KMS and HM techniques at *t=0.25 days*

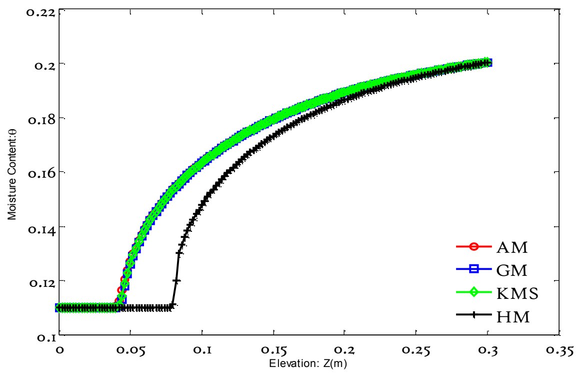

Figure 6. Water content profiles of AM, GM, KMS and HM techniques at *t=0.25 days.*

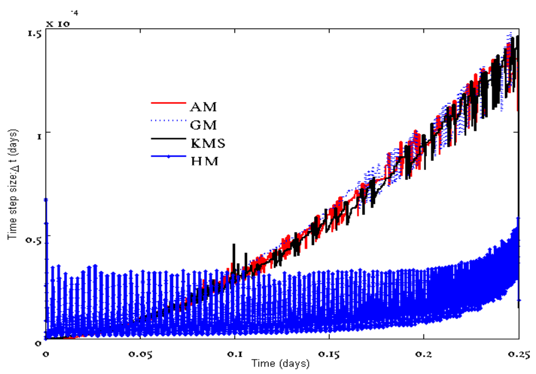

Figure 7. Time step variations of various schemes throughout the simulation.

TABLE 1. Comparison of computational statistics for various estimation techniques

	AM	GM	KMS	HM
No. of successful steps	4896	4773	5034	18788
No. of failed attempts	117	61	122	1131
No. of function evaluations	12039	12164	12599	41418
No. of partial derivatives	19	20	19	66
No. LU decompositions	501	356	509	2686
No. of Solutions of linear systems	9188	9163	9748	31517
CPU (s)	19.43	23.00	20.51	154.85

The evolution of time step (see Figure 7) variation of AM, GM and KMS shows a smooth increase of the step size. The step size evolution produced by the automatic adaptive scheme is quite intuitive. Throughout the simulation, the profiles are characterized by very rapid and highly nonlinear moisture flows due to abrupt forcing. Except for the case of HM, a dramatic rise in step size takes place as the infiltration front reaches the end of the soil column. Therefore the most robust combination of interblock permeability estimation are the AM, GM and KMS for this test case.

5. 2. Test Case 2 In order to evaluate the influence of the different conductivity averaging approaches, a vertical infiltration problem in a *60cm* soil will be solved. This soil column is parameterized using the van Genuchten relationships with $K_s = 0.00922\ cm/s$, $\alpha = 0.0035/cm$, $\theta_r = 0.102$, $\theta_s = 0.368$, and $n = 2$. A vertical discretization of 0.6 cm is used. The Dirichlet boundary conditions are $\psi(0,\ t) = -75\ cm$ and $\psi(60,\ t) = -1000\ cm$. The initial pressure profile is specified as:

$$\psi(Z,t) = \begin{cases} -1000, & Z \geq 06 \\ -75 - \frac{925}{0.6} Z, & 0 \leq Z < 0.6 \end{cases}$$

These forcing conditions lead to the development of a sharp infiltration front and induce large gradients in the solution. This type of problem provides a rigorous test case for time integrators and is well suited for the analysis of numerical convergence and efficiency. We used analytical differentiation of the soil characteristic curves. The soil moisture characteristic curves of hydraulic conductivity profiles for the various interblock estimation techniques by the van Genuchten model is shown in Figure 8. The propagation of pressure head and moisture content at the time 20000s, 40000s, 60000s, 80000s and 100000s through the problem domain with arithmetic estimation technique obtained by automatic adaptive time stepping is presented in Figures 9 and 10, respectively, which are in good agreement with the published studies [4, 41-43].

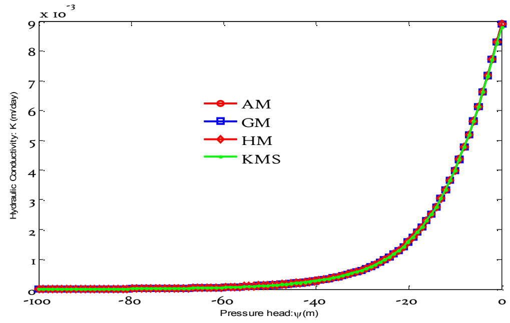

Figure 8. Hydraulic conductivity profiles for four averaging schemes

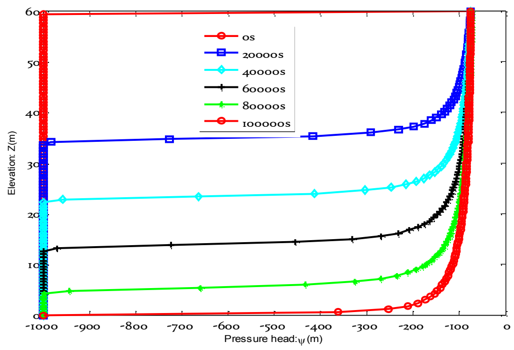

Figure 9. Pressure head profiles of AM averaging technique

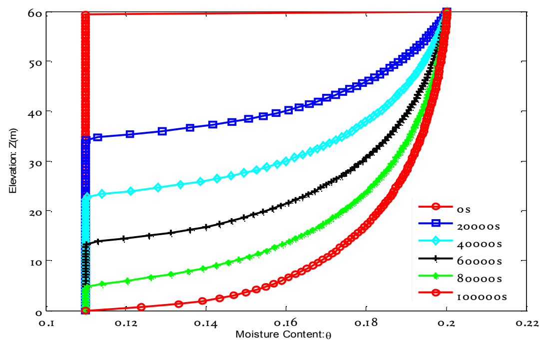

Figure 10. Water content profiles of AM averaging technique.

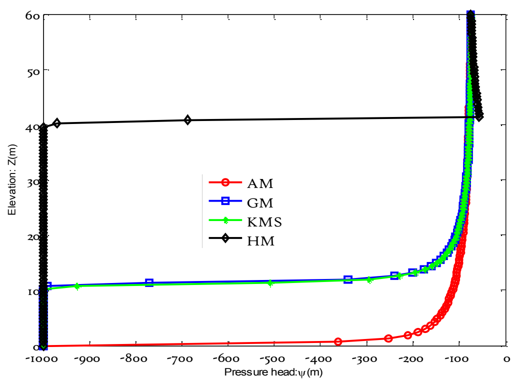

Figure 11. Pressure head profiles of AM, GM, KMS and HM techniques at *t=100000s.*

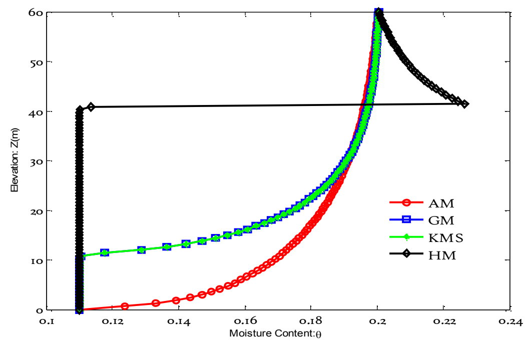

Figure 12. Water content profiles AM, GM, KMS and HM techniques at *t=100000s.*

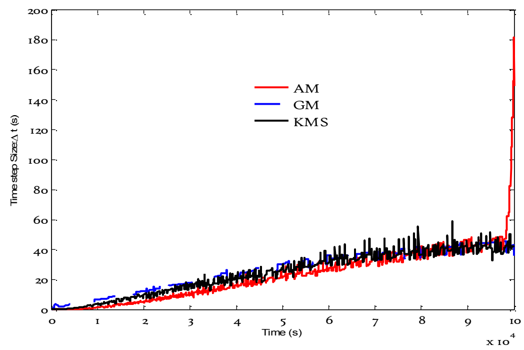

Figure 13. Time step variations of various schemes throughout the simulation.

TABLE 2. Comparison of computational statistics for various estimation techniques

	AM	GM	KMS	HM
No. of successful steps	4435	3727	4144	Div
No. of failed attempts	127	38	143	Div
No. of function evaluations	9849	8318	8773	Div
No. of partial derivatives	14	11	11	Div
No. LU decompositions	526	243	525	Div
No. of Solutions of linear systems	8847	7217	7672	Div
CPU (s)	13.26	12.13	10.47	Div

*Div=Divergent

Figures 11 and 12 show the pressure head and moisture content profiles for various interblock estimation techniques at the end of the simulation for this problem. In these two figures, we see that simulation is noticeably less accurate within the framework of GM and KMS techniques. Weighting scheme HM completely diverges for this test problem. The similar behavior is shown by the GM and KMS averaging approaches. Based on the results of this simulation, it is concluded that the best selection for this test case is arithmetic weighting scheme.

Simulation statistics for various runs are summarized in Table 2. The algorithm efficiency can be assessed also on the basis of actual accuracy for a given computational cost. The total number of iterations can be used as the measure of computational effort since the CPU time is governed by the total number of matrix inversions, rather than the number of time steps. Least amount of computational efforts (the CPU time and the total number of iterations) using the proposed criterion (AM, GM, KMS) is required.

It is of practical interest to examine the pattern of step size variation, shown in Figure 13. The number of time step is important since the time size may be strongly influenced by the convergence of the nonlinear solver. It is seen that, cost of the automatic time step selection is very small at the beginning of the simulation for all the runs but rapidly increases at the end of the simulation along with arithmetic approximation. Behavior of HM is not included here as the cause of divergence.

6. CONCLUSIONS

The study presents various estimating methods of interblock permeability for the numerical solution of the mixed form of Richards' equation, which produces consistently superior results. Numerical trails demonstrate that the hydraulic conductivity plays an important role to solve Richards' equation accurately. For example, numerical results presented for the first test case shows that the conductivity averaging schemes based on AM, GM, and KMS perform generally better than HM. In contrast, schemes based on GM and KMS averaging are shown to be sufficiently less accurate in test case 2. Hence, it can be concluded that the averaging techniques are not universal, it is highly problem dependent, i.e., averaging technique is highly dependent on the shape of the conductivity function, initial and boundary conditions of the problem and the discretization of the problem domain. In this study, we deal only with the application of the one-dimensional vertical Richards' equation to unsaturated flow problems in initially dry and homogeneous soils. In principle, however, these weighting averaging approximations can also be used to analyze flow in more complex and realistic situations such as multidimensional flow in heterogeneous soils.

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Selection of Intermodal Conductivity Averaging Scheme for Unsaturated Flow in Homogeneous Media

M. Sayful Islam

Department of Mathematics, Shahjalal University of Science & Technology, Sylhet, Bangladesh

PAPER INFO

Paper history:
Received 08 October 2014
Received in revised form 29 December2014
Accepted 29 January 2015

Keywords:
Richards' Equation
Variably Saturated Flow
Internodal Conductivity
Infiltration
Finite Difference

چکیده

روشهای حل غیر خطی برای حل عددی جریان آب در خاکهای اشباع شده احتمالا با مشکلات متعددی همراه است. عوامل مختلفی می توانند باعث افزایش این مشکلات شوند که از جمله آنها شرایط اولیه بسیار خشک است که موجب گرادیان فشار با شیب زیاد و تغییرات شدید هدایت هیدرولیکی در قسمت مرطوب در طی نفوذ آب می شود. بنابراین، روش متوسط گیری که برای محاسبه هدایت هیدرولیکی بین دو نقطه مجاور در آرایه محاسباتی استفاده می شود یکی از مسائل مهمی است که روی دقت حل عددی معادلات جریان غیر اشباع تک-بعدی مانند معادله ریچارد تاثیر می گذارد. الگوهای متوسط گیری مختلفی از جمله آریتمیک، ژئومتریک، هارمونیک و اشباع متوسط آریتمیک در متون برای خاکهای همگن ارائه شده است. الگوهای عددی به دست آمده از لحاظ دقت و زمان محاسبه مورد بررسی قرار می گیرند. ملاحظه می شود که الگوی متوسط گیری در چارچوب روش اریتمیک برای تعدادی از موارد بررسی شده به طور مطلوبی به روشهای دیگر نزدیک است.

doi: *10.5829/idosi.ije.2015.28.04a.01*