AN ALTERNATIVE FORMULATION FOR UNSATURATED FLOW

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ABSTRACT
Different forms of the moisture transport equations can lead to significantly different results for the same problem. The pressure head form usually suffers from large mass balance errors while the moisture content form, conserves mass perfectly but has difficulty handling material boundaries and near saturation conditions. This paper presents a conservative mixed formulation in which the discharge velocity and pressure head are the primary field variables. Solutions from the proposed formulation are compared with that of a mixed and pressure head form of Richards equation for infiltration into homogenous and heterogeneous unsaturated soil columns.

RÉSUMÉ
Différentes formes des équations de transfert d'humidité peuvent donner des résultats significativement différents pour un même problème. L'allure de la pression superficielle est entachée par de grandes erreurs dues à la balance de masse, alors que la forme de la courbe d'humidité conserve parfaitement l'effet de masse, mais supporte moins bien les conditions limites des matériaux et les conditions proche de la saturation. Cet article présente une formulation mixte et conservative dans laquelle la vitesse d'écoulement et la pression superficielle sont les variables de base observées. Des résultats obtenus de la formulation proposée sont comparés avec ceux d'une formulation mixte et une formulation de la pression superficielle dérivée de l'équation de Richard pour des scénarios d'infiltration dans des colonnes de sol non-saturées homogènes et hétérogènes.

1. INTRODUCTION

Water movement in the unsaturated zone, together with its water holding capacity is very important for the many branches of science and engineering such as soil and fluid mechanics, agricultural and environmental engineering. Moisture movement in the vadose zone is governed by the Richards equation expressing Darcy's Law and Law of mass conservation. This equation has been written in three different forms: the "ψ-based" form, the "θ-based" form, and the "mixed-form". Analytical and simplified solutions are only available for very simple unsaturated flow systems with relatively simple initial and boundary conditions. Numerous numerical models have been developed for the solution of the Richards equation using finite difference, finite element, and integrated finite difference methods. However the numerical approximations based on the different forms of the Richards equation can lead to significantly different results for the same problem.

This paper explores the use of a conservative mixed formulation in which the 'discharge' velocity and pressure head are the primary field variables. Solutions from the proposed formulation are compared with that of a standard mixed formulation for different scenarios of infiltration into homogenous and heterogeneous unsaturated medium. The case of evaporation from saturated soil and change in location of the phreatic surface are also considered.

2. FIELD EQUATIONS

This section presents the equations most often encountered in groundwater flow. We begin by providing the key definitions of variables then proceed to take a close look at Darcy's equation for saturated flow, as well as that of mass balance. Finally, the various mathematical descriptions for unsaturated flow are summarized.

2.1 Basic Definitions

The energy state of groundwater relative to some datum is most often expressed in terms of total head *h*, which is the sum of the pressure head ψ and elevation head *z*; i.e.,

$$h = \psi + z \qquad [1]$$

which may also be written for the case of saturated soil as

$$h = \frac{u}{\gamma_w} + z \qquad [2]$$

with *u* and γ_w being the pore pressure and unit weight of the water, respectively.

The degree of saturation S_r of the soil may be expressed in terms of the volumetric moisture content θ and porosity n as

$$S_r = \frac{\theta}{n} = \frac{V_w}{V_t}\frac{V_t}{V_v} \qquad [3]$$

with V_w, V_v and V_t being the volume of water, void and total, respectively. For a soil that is saturated, the specific storage S_s is related to the compressibility of the soil skeleton α and that of the water β via

$$S_s = \gamma_w(\alpha + n\beta) \qquad [4]$$

The specific moisture capacity C, which is derived from the soil-moisture characteristic curve, and soil-water diffusivity D are given by

$$C = \frac{d\theta}{d\psi} \quad \text{and} \quad D = \frac{K}{C} \qquad [5]$$

in which K represents the hydraulic conductivity.

2.2 Transient Saturated Flow

Let us begin with mass balance assuming that the density of the fluid in the pores remains relatively constant. The conservation of mass for transient flow in a saturated porous medium is given by

$$\nabla^T \mathbf{q} = -S_s \frac{\partial h}{\partial t} \qquad [6]$$

where t denotes time, the superscript T is the transpose operator and the left hand side is the divergence of the discharge velocity $\mathbf{q}$, which is given by Darcy's relation

$$\mathbf{q} = -K\nabla h \qquad [7]$$

which for the current form assumes isotropy. One can substitute this equation into eq. 6 to obtain an expression in terms of total head; i.e.,

$$\nabla^T (K\nabla h) = S_s \frac{\partial h}{\partial t}. \qquad [8]$$

At this point, it is advantageous to take a closer look at the interpretation of eq. 7, which may be expressed as

$$-\nabla p - \left(\gamma_w \nabla z + \frac{\gamma_w}{K}\mathbf{q}\right) = \mathbf{0} \qquad [9]$$

An examination of this equation reveals that it is a statement of fluid equilibrium, in which the first term in brackets corresponds to the unit gravitational body force and the second term is the drag associated with the interaction of the moving fluid and soil particles.

2.3 Transient Unsaturated Flow

Rather than dealing with pressure, we can express eq. 9 in terms of pressure head; i.e.,

$$-\nabla \psi - \left(\nabla z + \frac{\mathbf{q}}{K}\right) = \mathbf{0}. \qquad [10]$$

This form is more convenient for the analysis of unsaturated groundwater flow within rigid porous media. It is important to recognize that the hydraulic conductivity is an explicit function of the pressure head or volumetric moisture content. Drawing parallels with eq. 9, this equation may be viewed as a statement of equilibrium, with the fluid phase assumed to be continuous.

The mass balance equation corresponding to eq. 10 is

$$\nabla^T \mathbf{q} = -\frac{\partial \theta}{\partial t} = -C\frac{\partial \psi}{\partial t}. \qquad [11]$$

Implicit in this expression is the assumption that the change in the degree of saturation is more important than changes in fluid density or porosity. Depending on how the equations are manipulated, we can have the well-known forms

$$\nabla^T (K\nabla(\psi + z)) = -C\frac{\partial \psi}{\partial t} \qquad [12]$$

or

$$\nabla^T (D\nabla\theta) + \frac{\partial K}{\partial z} = \frac{\partial \theta}{\partial t}. \qquad [13]$$

It is important to recognize that both of these forms assume that the major form of moisture transport is due to the advective movement of the liquid phase and that osmotic pressures can be neglected.

3. NUMERICAL IMPLEMENTATION

The procedures for converting eq.'s 12 and 13 to forms for numerical implementation are well established and the reader is referred to Zienkiewicz and Taylor (1989) for details. This section is devoted to discussing the advantages and disadvantages of each formulation, with the section that follows providing details on the development of a mixed finite element procedure.

3.1 ψ and θ Formulations

The various forms of the transient unsaturated flow equation are parabolic partial differential equations, which are highly non linear due to the dependence of specific moisture capacity and hydraulic conductivity on the pressure head. Owing to the non-linear nature of the equations, analytical solutions are only possible in special cases. The numerical approximations for both the moisture content and the pressure head formulations involve the use of finite difference or finite element techniques in the spatial domain, and simple one-step time marching algorithms in the time domain. For any Euler method other than the explicit forward method, non-linear algebraic equations result and some linearization and/or iteration procedure must be used to solve the discrete equations.

One of the attractions of using the θ-based equation is the fact that the discrete approximation to the equation can be formulated using the finite element or finite difference method such that the approximation is perfectly mass conservative. However such approximations to the ψ-based formulations usually result in large mass balance errors (Milly 1988, Celia et al. 1990). The reason for poor mass balance in ψ-based algorithms stems from the time derivative term. While $\partial\theta/\partial t$ and $C\,\partial\psi/\partial t$ are mathematically equivalent in the continuous partial differential equation their discrete analogs are not. Although the algorithms based on θ-based equation provide more accurate mass conservation, the equation degenerates once the system or part of the system becomes saturated as $D(\theta)\rightarrow\infty$. Another problem with the θ-based equation stems from the term $\nabla\theta$, which becomes discontinuous at the material interfaces due to different moisture retention capacities of different materials.

These observations regarding the θ-based and ψ-based algorithms have inspired development of a mixed form for the equation. In this formulation the term provides the mass conservation property inherent in the θ-based algorithms, and the solution is developed in terms of pressure head. This avoids problems with saturation and material interfaces. One of the first authors to combine mixed form of the Richards equation and Newton iteration was Brutsaert (1971). He presented effectiveness of his technique in dealing with sharp wetting fronts in initially dry soils. More recently Bouloutas (1989) and Celia et al. (1990) have solved the mixed form of the Richards equation using modified Picard iteration and a preconditioned conjugate gradient solver for sharp wetting fronts in initially very dry soils and have shown excellent mass conservation.

Kirkland et al. (1992) presented a Flux-Updating Iterative Gradient Algorithm for the solution of Richards equation. In their algorithm they solve the Pressure head form of the Richards equation using finite difference. Once the estimates of pressure head at all locations are obtained, Fluxes are calculated at each individual node by invoking Darcy law at the nodes. These fluxes are then used to calculate water contents using the conservation of mass. The estimates of the water contents are used with the water retention relationship to calculate new estimates of pressure head. This algorithm is mass conservative in the sense that it avoids the finite difference approximation of the term $C\,\partial\psi/\partial t$ as fluxes are used to update water contents. However the algorithm becomes unstable at saturated-unsaturated interface. This can be avoided by rejecting the new estimate of the water content of a particular node if it is adjacent to a saturated node. This adds small mass balance errors but is necessary to improve stability.

3.2 q - ψ Mixed Formulation

Let us for the moment consider the saturated case. If we were to interpret eq. 9 as a statement of equilibrium, the standard approach would be to multiply this expression by a virtual velocity $\boldsymbol{\delta}\mathbf{q}$, integrate over the domain and then integrate the pressure term by parts to obtain a weak statement of equilibrium. eq. 6 would be multiplied by a virtual pressure $\boldsymbol{\delta}p$ before integrating over the domain. This philosophy is followed for the unsaturated flow equations.

Taking eq. 10 and multiplying it by $\boldsymbol{\delta}\mathbf{q}$, one has

$$\int_V \boldsymbol{\delta}\mathbf{q}^T\left(\nabla\psi+\nabla z+\frac{\mathbf{q}}{K}\right)dV=0 \qquad [14]$$

or after applying the divergence theorem

$$\int_V\left(-\nabla^T\boldsymbol{\delta}\mathbf{q}\psi+\boldsymbol{\delta}\mathbf{q}^T\nabla z+\boldsymbol{\delta}\mathbf{q}^T\frac{\mathbf{q}}{K}\right)dV+\int_S(\boldsymbol{\delta}\mathbf{q}\psi)^T\mathbf{n}\,dS=0 \qquad [15]$$

with $\mathbf{n}$ referring to the normal of the surface S where the pressure head is specified. The weak form for mass balance is

$$\int_V \boldsymbol{\delta}\psi\left(\nabla^T\mathbf{q}+C\frac{\partial\psi}{\partial t}\right)dV=0\,. \qquad [16]$$

Given that stresses are related to the gradients of displacement or velocity, the interpolation of the pressure head should be one order less than that of velocity **q**. If we use a linear variation of **q**, then ψ within an element is constant. It should be noted here that the head need not be continuous between elements and that the specification of pressure head enters as a natural boundary condition similar to a surface traction. Assuming constant pressure head within an element, the discretized form of

$$\nabla^T \mathbf{q} + C\frac{\partial \psi}{\partial t} = 0 \qquad [17]$$

can be applied directly.

3.3 One-Dimensional Implicit Formulation

The discretized form of eq.'s 15 and 17 are developed on the element level for one-dimensional implicit case. Let us first consider the mass balance equation. Given linear variation in velocity and constant ψ, the pressure head $\psi_{t+\Delta t}$ at the end of time interval Δt

$$\psi_{t+\Delta t} = \psi_t - \frac{\Delta t}{C\ell}\left(q_2 - q_1\right)_{t+\Delta t} \qquad [18]$$

where ℓ is the length of the element, and q_1 and q_2 are nodal discharges corresponding to the end of the interval. The updated moisture content $\theta_{t+\Delta t}$ is

$$\theta_{t+\Delta t} = \theta_t - \frac{\Delta t\left(q_2 - q_1\right)_{t+\Delta t}}{\ell}. \qquad [19]$$

As we can see from this equation, the moisture content is related directly to the discharge, thus the quantity is conserved.

Assuming a typical element, and observing that ψ in eq. 15 corresponds to the value at the end of the time step, we have for single element

$$\left[\frac{\Delta t}{C\ell}\begin{bmatrix}1 & -1\\ -1 & 1\end{bmatrix} + \frac{\ell}{6K}\begin{bmatrix}2 & 1\\ 1 & 2\end{bmatrix}\right]\begin{Bmatrix}q_1\\ q_2\end{Bmatrix}_{t+\Delta t} = \psi_t\begin{Bmatrix}-1\\ 1\end{Bmatrix} - \frac{\ell}{2}\begin{Bmatrix}1\\ 1\end{Bmatrix}. \qquad [20]$$

When introducing more elements it is necessary to add the proper contributions from each element on both sides of the equation. From a numerical point of view, it may be necessary to implement an iterative improvement scheme to minimize the loss of significant digits since the values for *C* and *K* can vary several orders of magnitude.

There is one more observation to be made here. Implicitly it has been assumed that the only moisture transfer is due to the flux of liquid water. Given that the flux is continuous and that information pertaining to the mode of transport is internal to an element, as is the potential function (head), it is possible to allow for a different mode within each element (cell).

4. NUMERICAL EXAMPLES

In this section, examples are presented, which demonstrate the capability of the proposed analysis framework to model moisture transfer. In the first example, the focus is on being able to predict, not only the variation in head and water content as a function of depth, but also the location of the phreatic surface as evaporation takes place at the surface. Since we are dealing with a saturated medium for this problem, consolidation is also taken into account. The emphasis in the problems that follow is the treatment of unsaturated flow for the case of infiltration

4.1 Moisture Transfer in a Consolidating Medium

Let us consider a situation where the bottom of a quarry is filled within a very short period with 2 m of soft fine-grained till with initial water content (by mass) of 70% and unit weight of 16 kN/m^3. Based on tests completed in the laboratory, the hydraulic conductivity is approximately 0.0005 m/hr. Site conditions are such that the moisture loss is by evaporation at the upper horizontal surface at an average rate of 0.0001 m/hr.

Given the short duration of construction, the excess pore pressure varies linearly with depth. To take into account consolidation, the equilibrium of the solid phase must also be considered. Following the procedure outlined by Stolle et al. (1999), the field equations describing the physics may be combined to yield

$$\frac{\partial \sigma'}{\partial t} + \gamma' = \frac{\gamma_w}{K}\frac{\partial q}{\partial t} \qquad [21]$$

where γ' and σ' are the buoyant unit weight and effective stress, respectively, and *q* represents the vertical discharge velocity, with the other terms the same as described previously. Taking into account the incompressibility of the water

$$\frac{\partial \sigma'}{\partial t} = -E\frac{\partial q}{\partial z} \qquad [22]$$

where $E = 250 + 20\sigma'$ kPa is the elastic modulus. Implicit in this equation is the assumption that the one-dimensional strain rate is directly related to the discharge gradient. Figures 1 and 2 show the variation of pore pressure and water contents with depth at various stages after the clay was placed.

Referring to Figure 1, one observes that the rate of pore pressure increase with depth decreases once the excess pressure dissipates, as one might expect. Initially, the water is supporting the total load and as water is squeezed out, the soil skeleton takes more and more of the load, thus causing the pore pressures to decrease. At later stages when the pore pressure at the surface becomes negative, the water in the upper zone is in suction, increasing the effective stress above values dictated by the buoyant unit weight alone. The settlement of the surface after 864 hrs is approximately 8.6 cm. An important observation is that the location of the phreatic surface is predicted as part of the solution. When dealing with pressure head formulations, a reference head must be specified. For constant K this does not present difficulties. On the other hand, problems arise if the hydraulic conductivity is a function of head.

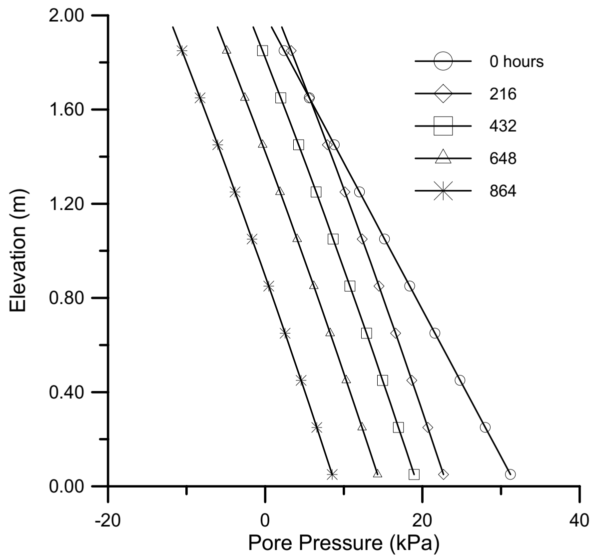

Figure 1. Pore pressure as a function of elevation.

As one might expect, the water content w of the soil mass decreases with time. An interesting observation when examining the variation of water content (216 hrs) with elevation is the temporary increase in w near the surface. This increase is due to consolidation forcing the water upwards faster than it can be evaporated away. For the situation where there may be a gentle slope and surface runoff can occur, provisions must be introduced to allow for discharge gradients that exceed evaporation. These simulations do not accommodate this possibility.

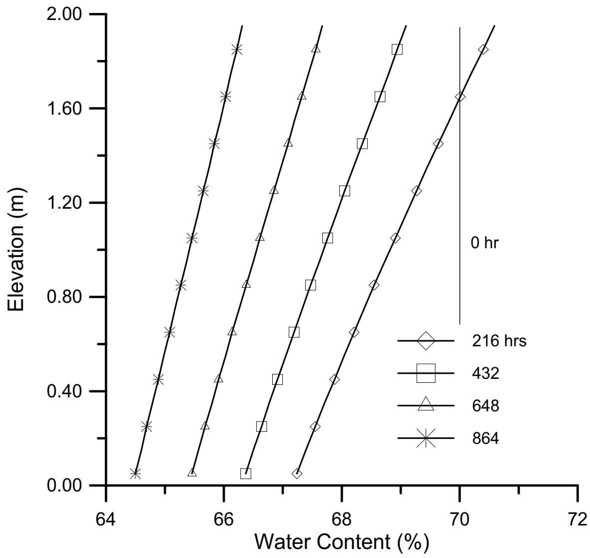

Figure 2. Water content as a function of elevation.

4.2 Infiltration in Unsaturated Soil

The proposed unsaturated finite element model is demonstrated here by comparing its predictions with those from HYDRUS 5.0 (Vogel et al. 1996) for a problem chosen from the literature. The HYDRUS code uses the mixed form of the Richards equation and the mass conservative algorithm developed by Celia et al. (1990), who also present results for a simulation dealing with water infiltration in a 100-cm column of homogenous soil in which constant pressure head is maintained at the top (ψ = -75 cm) and at the bottom (ψ = -1000 cm). The initial pressure head was -1000 cm over the entire depth.

The soil properties, obtained from a field measurement at a New Mexico site, are represented by the empirical expression

$$\theta(\psi) = \frac{\theta_s - \theta_r}{\left[1 + \left(\alpha|\psi|\right)^n\right]^m} + \theta_r \qquad [23]$$

$$K(\psi) = K_S \frac{\left\{1 + \left(\alpha|\psi|\right)^{n-1}\left[\left[1 + \left(\alpha|\psi|\right)^n\right]^{-m}\right]\right\}^2}{\left[1 + \left(\alpha|\psi|\right)^n\right]^{\frac{m}{2}}} \qquad [24]$$

where K_S (= 0.00922 cm/s) is the saturated hydraulic conductivity, θ_s (= 0.368) and θ_r (= 0.102) are the saturated and residual moisture contents, respectively, and the values of the other parameters of these relations are α = 0.0335, n = 2 and m = 0.5.

The simulations with the proposed model were completed using an implicit time marching scheme. No attempt was made to iterate within a time step to minimize the residual. Any residual that was incorporated into the calculation of the discharge velocities for the following time step was to reduce algorithmic drifting. It should be noted that the pressure heads were specified via a 'natural' boundary condition.

Figures 3 and 4 show the steady state pressure head and moisture content variations with depth, respectively. An examination of the predictions indicates that the proposed model is capable of modeling the infiltration phenomenon. Although reasonable agreement was possible when using equivalent element spacing, in order to obtain good agreement, twice as many elements were required for the simulation with the q - ψ mixed formulation. This may be due to the use of lower order interpolation for head in the proposed scheme.

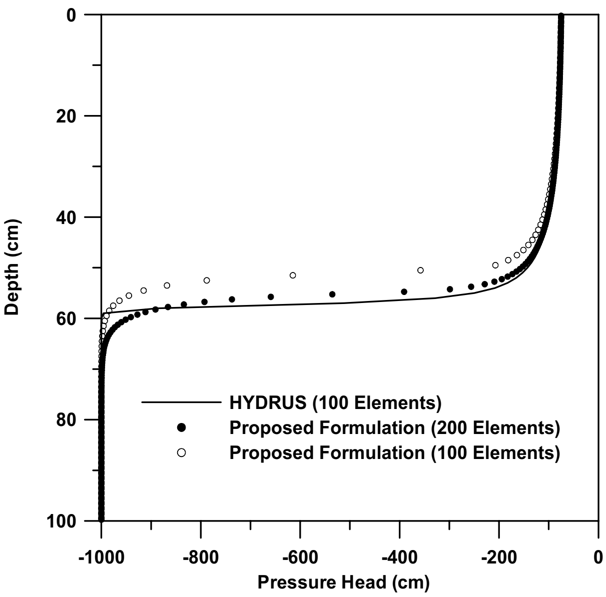

Figure 3. Pressure head as a function of depth.

4.3 Comparison with Pressure Head Formulation

In this section the proposed q-ψ mixed form is compared with finite element and finite difference approximation of pressure head form of Richards equation. The test consists of infiltration into a homogenous unsaturated sand column with height 120 cm. The constitutive relationships for sand used are

$$\theta = \frac{\alpha(\theta_s - \theta_r)}{\alpha + |\psi|^{\gamma}} + \theta_r \qquad [25]$$

$$k = k_s \frac{A}{A + |\psi|^{\beta}} \qquad [26]$$

as reported by Haverkamp et al. (1977). The value of the parameters are K_s = 9.440 10^{-3} cm/s, A = 1.175 106, α = 1.611 106, β = 4.474, γ = 3.9600, θ_s = 0.2870, θ_r = 0.0750. The initial and boundary conditions are given as:
ψ(z,0) = -100 cm (θ = 0.07903 cm^3/cm^3); ψ(0,t) = -20 cm (θ = 0.269 cm^3/cm^3); and ψ(L,t) = -100 cm .

The moisture content profiles predicted with the proposed model and the results reported by Gottaardi and Ventutelli (1993) using their computer program Richards are shown in Fig. 5. It can be seen that there is a good agreement between the results of the proposed model and those of the finite difference and finite element formulations of pressure head form of Richards equation

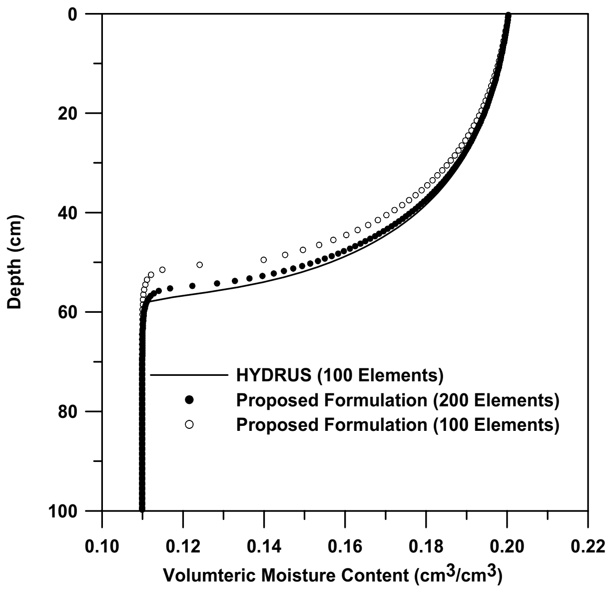

Figure 4. Moisture content as a function of depth.

4.4 Infiltration in to an unsaturated layered Profile

The proposed model was used to simulate an infiltration event regarding an unsaturated layered column of height 75 cm as reported by Gottaardi and Ventutelli (1993). Starting from the top of the column the profile consisted of sequencing: sand, Glendale clay loam, Berino loamy fine sand, Yolo light clay and then sand. The constitutive relationships for Sand are given by eq.'s 25 and 26 and. For Berino loamy fine sand, and Glendale clay loam are given by eq.'s 23 and 24. The constitutive relationships for Yolo light clay are given by

$$\theta = \frac{\alpha(\theta_s - \theta_r)}{\alpha + \left(|\ln|h|^{\gamma}\right)} + \theta_r \quad [27]$$

$$k = k_s \frac{A}{A + |h|^{\beta}} \quad [28]$$

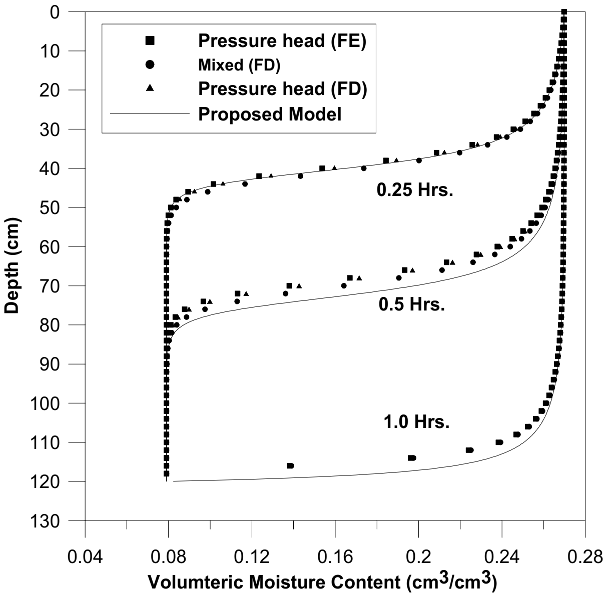

Figure 5. Comparison of solutions from various models

The values of parameters for the soils mentioned above are summarized in Table 1. It should be noted that these typical high and low permeability soils have been used extensively in soil science literature see, e.g., Haverkamp et al. (1977) and Hills et al. (1989). The initial and boundary conditions for the test at constant pressure head were: ψ(z,0) = -600 cm; ψ(0,t) = -20 cm ; and ψ(L,t) = -600 cm

In the situation of layered soils, the pressure head must be continuous across the material interface while the water content needs not to be. The pressure head and water content profiles obtained from proposed formulation show a good agreement with the results reported by Gottaardi and Ventutelli (1993) as can be seen in Figures 6 and 7.

5. CONCLUDING REMARKS

This paper proposes a non-conventional algorithm for finding the solution to unsaturated flow problems. The scheme parallels that found in the literature for saturated flow, in which the 'discharge' velocity is the primitive variable, with head and moisture content being secondary quantities derived from the velocity field. Given that the moisture content is determined directly from the velocity field, mass is conserved. The proposed non-conventional algorithm compares well with other various forms of Richards equation for both homogenous and heterogeneous profiles.

At this stage of the development, the model is incomplete. Issues requiring investigation include, for example, the use of lumped mass and iterative refinement to improve numerical efficiency and reduce the size of residual when using larger time steps.

Table 1. Parameters for soils used in simulation of infiltration in to layered profile

Soil	K_s (cm/sec)	A	α	β	γ/n	θ_s	θ_r
Sand	0.00944	1176000	1611000	4.47	3.96	0.287	0.075
Yolo	0.00001	125	739	1.77	4	0.495	0.124
Berino	0.00626	-	0	-	2.24	0.366	0.029
Glendale	0.00015	-	0	-	1.4	0.469	0.106

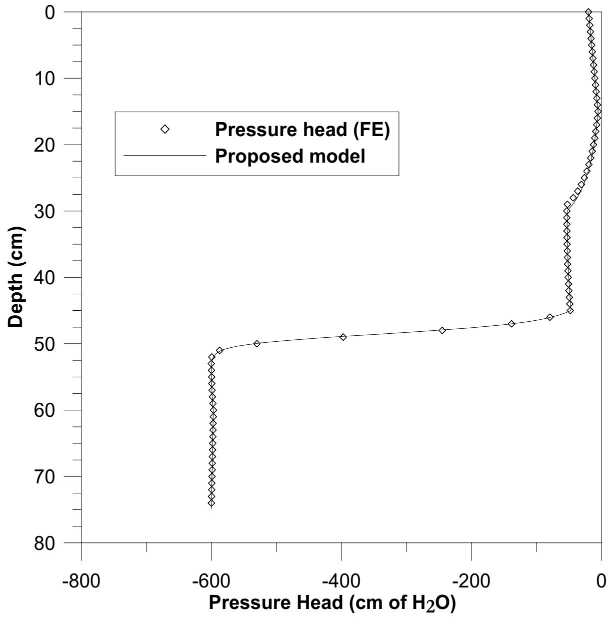

Figure 6. Comparison of ψ for layered case

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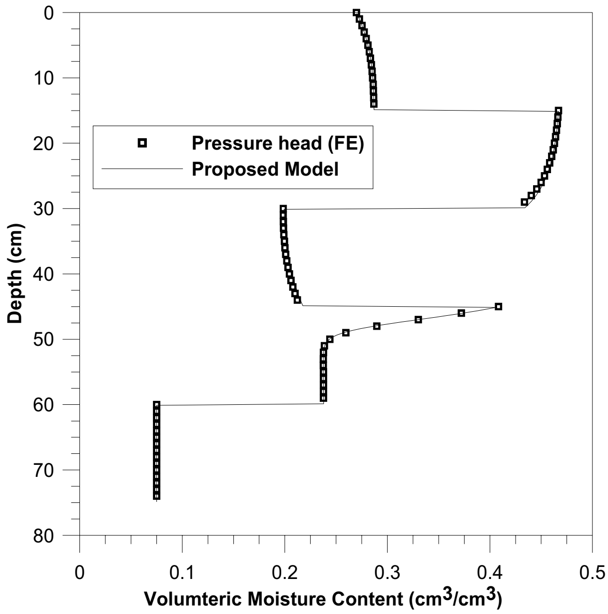

Figure 7. Comparison of θ for layered case