Finite element for Richards’ equation in porous rocks

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Abstract. The interaction processes of water movement and environment have several aspects important to engineering and geology, which motivate a large amount of research all over the world. As computers with larger capacity become available and affordable, several simplifications used in the past have become meaningless, and nonlinear complex phenomena like unsaturated flow can be processed in affordable machines. The reduction of water flow capacity of filters and drains in embankments due to unsaturated zones, and the environmental problems of remediation of contaminated zones in porous rock masses at the vadose zone are examples of special problems in which advanced modeling should be applied to avoid misleading conclusions or dreadful consequences. The unsaturated flux can also be important in understanding the influence of humidity in the bowing phenomenon in calcitic marbles, since laboratory tests have shown different evolutions of this pathology in partially saturated samples and in completely wet or dry samples. Moreover, this formulation also has important application in building envelope modeling, like in evaporative roofs which enhance thermal comfort in hot weather. To increase the understanding of unsaturated problems, this paper presents a finite element formulation for applications in unsaturated flow in stiff porous media, like sedimentary rocks or concrete. The formulation is based on Richards’ equation for one-dimensional flows and it includes a linear interpolation of suction, as well as an arbitrary implicit parameter.

1. Introduction

Water dynamic in geomaterials has long challenged engineers due to the complexity of this phenomenon and its importance to engineering and geology fields. Complex phenomena, such as the consolidation of soft soils [1, 2], usually assume saturated conditions to evaluate the water flow. However, if the layers of soft soils are settled in areas where the phreatic level varies along the year, the fully saturated condition might not be representative anymore. Problems for which the simplification previously mentioned should not be applied are not so rare in geotechnical engineering, and the misuse of saturated materials formulations can lead to catastrophic events.

It is known that a critical step in dam operation is the first filling of the reservoir because loads on the geotechnical structures are increasing continuously, and instrumentation data must agree with those predicted in geotechnical design [3], including filter and drains. In clay-core rockfill dams or earthen dams, the clay is the head material responsible for keeping the reservoir filled. In the beginning, the material is in dry or unsaturated condition, and, as soon as the flownet starts to take place, the saturated state under the phreatic line is reached. During this process, the piezometric readings must be monitored and the water flux in saturated and unsaturated conditions must be used to predict the values of this instrumentation.
Contaminated site remediation processes for porous rock masses or soils at the vadose zone are other examples where modeling of unsaturated conditions is necessary [4, 5, 6, 7]. In this case, the assumption of the saturated condition might lead to disastrous events if the contaminant remains in the ground after the treatment, or if it spreads over a larger area due to the diffusion process.

Due to the importance of this subject, a theoretical model of the nonlinear equation for water movement in unsaturated porous media, commonly known as Richards’ equation, is presented in this work considering unidimensional flux. Obviously, the 2-D and 3-D approaches are directly achieved just by considering the variation of the parameters referred to these degrees of freedom. The numerical approach using the spatial discretization via finite element method was used in this model. The main goal of this study is to provide a methodology to solve problems of unsaturated flux in porous media that can be implemented in any programming language.

2. Richards’ equation
Richards’ Equation [8] describes the unsaturated water flow in porous media. It is a nonlinear partial differential equation which renders its solution by traditional analytical methods elaborate. The unsaturated flow equation can be expressed in three forms: by capillary head (h-based), by water content (θ-based), or by the mixed form. This study takes into account the h-based form for one-dimension in an isotropic porous medium.

The equation of mass conservation for the transient water flow in a one-dimensional unsaturated porous medium can be represented by:

\[
\frac{\partial q_w}{\partial y} + \frac{\partial \theta_w}{\partial t} = 0,
\]

where \( q_w \) stands for the water flow, \( y \) stands for the vertical coordinate (assumed positive upward), and \( \theta_w \) stands for the volumetric water content and \( t \) is the time.

The water flow \( (q_w) \) is modeled by Darcy’s law,

\[
q_w = k_w \left( \frac{1}{\gamma_w} \frac{\partial \psi}{\partial y} - 1 \right),
\]

where \( k_w \) stands for the hydraulic conductivity, \( \gamma_w \) stands for the specific weight of water, and \( \psi \) stands for the matric suction.

Substituting Equation (2) into Equation (1), one has the mixed water content form of Richards’ Equation:

\[
\frac{\partial \theta_w}{\partial t} = \frac{\partial}{\partial y} \left[ k_w \frac{\partial (\psi - y)}{\partial y} \right].
\]

Even considering the various numerical solutions for Richards’ Equation in literature [9, 10, 11, 12, 13, 14], the search for robust numerical schemes is still subject of research in numerical methods. An extensive review of the numerical solutions of Richards’ Equation is presented by Farthing and Ogden [15].

In unsaturated porous media, the hydraulic conductivity \( (k_w) \) varies in space and time in function of matric suction \( (\psi) \). There are several constitutive relationships based on empiric models that govern the correlation between the hydraulic conductivity \( (k_w) \), the volumetric water content \( (\theta_w) \), and the matric suction \( (\psi) \). This study considers the model proposed by van Genuchten-Mualem [17, 16] in which the relationship between volumetric water content and matric suction can be expressed as

\[
\theta_w = \theta_r + \frac{\theta_s - \theta_r}{1 + (\alpha \psi)^n}.
\]
where $\theta_r$ stands for the residual water content, $\theta_s$ stands for the saturated water content, $\alpha$ stands for the air-entry parameter, and $n, m$ are the fitting parameters.

The relationship between hydraulic conductivity and the matric suction is represented by:

$$k_w = k_s \left[ \frac{1 - (\alpha \psi)^n - 1}{[1 + (\alpha \psi)^n]} \right]^2$$

(5)

where $k_s$ is the saturated hydraulic conductivity.

### 3. Discretization for one-dimensional finite element

For rigid porous materials, like sedimentary rocks and concrete, the water storage modulus ($m_w^2$), by definition, is:

$$m_w^2 = \frac{\partial \theta_w}{\partial \psi}$$

(6)

Applying the chain rule, one has:

$$\frac{\partial \theta_w}{\partial t} = m_w^2 \frac{\partial \psi}{\partial t}.$$  

(7)

Now, substituting Equation (7) into Equation (1), one gets:

$$\frac{\partial q_w}{\partial y} + m_w^2 \frac{\partial \psi}{\partial t} = 0.$$  

(8)

Using the Method of Weighted Residuals in Equation (8), its weak form is obtained,

$$\int_V u^* \cdot \left[ \frac{\partial q_w}{\partial y} + m_w^2 \frac{\partial \psi}{\partial t} \right] dV = 0,$$

(9)

where $u^*$ is the weighting function.

Integrating by parts the first term of Equation (9), one has:

$$\int_V \left( u^* \cdot \frac{\partial q_w}{\partial y} \right) dV = -\int_V \left( q_w \frac{\partial u^*}{\partial y} \right) dV + (u^* q_w)|^L_0.$$  

(10)

Substituting Equation (10) into (9), one gets:

$$\int_V \left( -q_w \frac{\partial u^*}{\partial y} + u^* m_w^2 \frac{\partial \psi}{\partial t} \right) dV + (u^* q_w)|^L_0 = 0.$$  

(11)

Recalling Equation (2), Equation (11) can be rewritten as:

$$\int_V \left( \frac{k_w}{\gamma_w} \frac{\partial u^*}{\partial y} + k_w \frac{\partial u^*}{\partial y} + u^* m_w^2 \frac{\partial \psi}{\partial t} \right) dV + (u^* q_w)|^L_0 = 0.$$  

(12)

Finally, isolating the matric suction on the left-hand side:

$$\int_V \left( \frac{k_w}{\gamma_w} \frac{\partial u^*}{\partial y} - u^* m_w^2 \frac{\partial \psi}{\partial t} \right) dV = (u^* q_w)|^L_0 + \int_V \left( \frac{k_w}{\gamma_w} \frac{\partial u^*}{\partial y} \right) dV.$$  

(13)
3.1. Temporal discretization

Bearing in mind that approximation by implicit time discretization was used in this study, time integrals are performed by the \( \theta \)-method [18]

\[
\int_{t}^{t+\Delta t} b(t) \, dt \approx \left\{ (1-\theta)b^t + \theta b^{t+\Delta t} \right\} \Delta t, \tag{14}
\]

where \( \theta \in [0,1] \) is a real number and \( b(t) \) is any time dependent variable of the formulation, for which

\[
b^t = b(t) \tag{15}
\]

\[
b^{t+\Delta t} = b(t + \Delta t). \tag{16}
\]

Time derivatives are approximated by simple central finite differences,

\[
\frac{\partial \psi}{\partial t} \approx \frac{\psi^{t+\Delta t} - \psi^t}{\Delta t}, \tag{17}
\]

where \( t \) is the initial instant, \( t + \Delta t \) is the final instant of the time interval.

Integrating the Equation (13) in the time domain, one has:

\[
\int_{t}^{t+\Delta t} \int_V \left( \frac{k_w}{\gamma_w} \frac{\partial u^*}{\partial y} \frac{\partial \psi}{\partial y} - u^* m_2^w \frac{\partial \psi}{\partial t} \right) \, dV \, dt = \int_{t}^{t+\Delta t} \left( u^* q_w \right)_0^L \, dt + \int_{t}^{t+\Delta t} \int_V \left( \frac{k_w}{\gamma_w} \frac{\partial u^*}{\partial y} \right) \, dV \, dt \tag{18}
\]

Now, integrals of Equation (18) are solved by Equations (14) and (17):

\[
\int_V \left( (1-\theta)\Delta t \frac{k_w}{\gamma_w} \frac{\partial u^*}{\partial y} \frac{\partial \psi}{\partial y} + \theta \Delta t \frac{k_w^{t+\Delta t}}{\gamma_w} \frac{\partial u^*}{\partial y} \frac{\partial \psi^{t+\Delta t}}{\partial y} \right) \, dV - \int_V \left( u^* \psi^{t+\Delta t} (1-\theta) m_2^{w,t} + \theta m_2^{w,t+\Delta t} \right) \, dV + \int_V \left( u^* \psi^t (1-\theta) m_2^{w,t} + \theta m_2^{w,t+\Delta t} \right) \, dV = \]

\[
u^* \cdot \Delta t ((1-\theta)q_w^t + \theta q_w^{t+\Delta t})|_0^L + \int_V \left( (1-\theta)\Delta t \frac{k_w}{\gamma_w} \frac{\partial u^*}{\partial y} + \theta \Delta t \frac{k_w^{t+\Delta t}}{\gamma_w} \frac{\partial u^*}{\partial y} \right) \, dV \tag{19}
\]

3.2. Spatial discretization

Derivative of matric suction \( \psi \) with respect to \( y \) is calculated as

\[
\frac{\partial \psi^t}{\partial y}(\xi) = \frac{\partial \xi}{\partial y} \frac{\partial \psi^t}{\partial \xi} = \frac{1}{L} (\psi_1^t + \psi_2^t), \tag{20}
\]

\[
\frac{\partial \psi^{t+\Delta t}}{\partial y}(\xi) = \frac{\partial \xi}{\partial y} \frac{\partial \psi^{t+\Delta t}}{\partial \xi} = \frac{1}{L} (-\psi_1^{t+\Delta t} + \psi_2^{t+\Delta t}), \tag{21}
\]

where \( L \) is the length of the element and \( \xi \) is the local coordinate.

Assuming that the matric suction \( \psi \) varies linearly in spatial domain, the integrals can be calculated using two points of the Gaussian quadrature \( (n=2) \). Therefore, it is possible to write \( m_2^w \) in function of matric suction \( \psi \) in the time \( t \) and \( t + \Delta t \) as a function of the values of \( m_2^w \) defined in the Gauss quadrature coordinates \( \xi_{p1} \) and \( \xi_{p2} \):

\[
m_{2,p1}^{w,t} = m_2^w (\psi_{p1}^t) \quad m_{2,p2}^{w,t} = m_2^w (\psi_{p2}^t) \tag{22}
\]

\[
m_{2,p1}^{w,t+\Delta t} = m_2^w (\psi_{p1}^{t+\Delta t}) \quad m_{2,p2}^{w,t+\Delta t} = m_2^w (\psi_{p2}^{t+\Delta t}) \tag{23}
\]
Using the Equations (20) to (23) to solve the volume integrals in Equation (19), and isolating $\psi^{t+\Delta t}$ on the left-hand side of the equation, one has:

\[
\frac{\Delta t}{\gamma_w} \frac{\partial u^*}{\partial y} \psi^{t+\Delta t}_2 \cdot \left\{ \frac{\theta}{2} \left[ k_w(\psi^{t+\Delta t}_{p1}) + k_w(\psi^{t+\Delta t}_{p2}) \right] \right\} - 
\frac{\Delta t}{\gamma_w} \frac{\partial u^*}{\partial y} \psi^{t+\Delta t}_1 \cdot \left\{ \frac{\theta}{2} \left[ k_w(\psi^{t+\Delta t}_{p1}) + k_w(\psi^{t+\Delta t}_{p2}) \right] \right\} - 
\frac{\Delta t}{2} \frac{u^{*}_{p1}}{2} \left( 1 + \frac{1}{\sqrt{3}} \right) \left[ \left( 1 - \theta \right) m^w_2 (\psi^{t}_{p1}) + \theta m^w_2 (\psi^{t+\Delta t}_{p1}) \right] + 
\frac{\Delta t}{2} \frac{u^{*}_{p2}}{2} \left( 1 - \frac{1}{\sqrt{3}} \right) \left[ \left( 1 - \theta \right) m^w_2 (\psi^{t}_{p2}) + \theta m^w_2 (\psi^{t+\Delta t}_{p2}) \right] - 
\frac{\Delta t}{2} \frac{\partial u^*}{\partial y} (\psi^t_2 - \psi^t_1) \left\{ \frac{1}{2} \left[ k_w(\psi^{t}_{p1}) + k_w(\psi^{t}_{p2}) \right] \right\} + u^{*}_{p2} \frac{\Delta t}{2} \left[ \left( 1 - \theta \right) q^w_2 + \theta q^{t+\Delta t}_2 \right] + 
\frac{\Delta t}{2} \frac{\partial u^*}{\partial y} \left( 1 - \theta \right) \frac{L}{2} \left[ k_w(\psi^{t}_{p1}) + k_w(\psi^{t}_{p2}) \right] + \Delta t \frac{\partial u^*}{\partial y} \left[ k_w(\psi^{t+\Delta t}_{p1}) + k_w(\psi^{t+\Delta t}_{p2}) \right] (24)
\]

Rearranging Equation (24) in matrix notation considering the global system, one has:

\[
\begin{bmatrix}
K_{11} & K_{12} \\
K_{21} & K_{22}
\end{bmatrix} \begin{bmatrix}
\psi^{t+\Delta t}_1 \\
\psi^{t+\Delta t}_2
\end{bmatrix} = \begin{bmatrix}
B_1 \\
B_2
\end{bmatrix} \tag{25}
\]

where $[K]$ is the stiffness matrix and $\{B\}$ is the load vector.

The element $K_{11}$ can be expressed by:

\[
K_{11} = \frac{\Delta t}{\gamma_w} L \left\{ \frac{\theta}{2} \left[ k_w(\psi^{t+\Delta t}_{p1}) + k_w(\psi^{t+\Delta t}_{p2}) \right] \right\} - 
\frac{L}{2} \left\{ \frac{2 + \sqrt{3}}{6} \right\} \left[ \left( 1 - \theta \right) m^w_2 (\psi^t_{p1}) + \theta m^w_2 (\psi^{t+\Delta t}_{p1}) \right] + 
\frac{L}{2} \left\{ \frac{2 - \sqrt{3}}{6} \right\} \left[ \left( 1 - \theta \right) m^w_2 (\psi^t_{p2}) + \theta m^w_2 (\psi^{t+\Delta t}_{p2}) \right] \tag{26}
\]

The element $K_{12}$ can be expressed by:

\[
K_{12} = -\frac{\Delta t}{\gamma_w} L \cdot \left\{ \frac{\theta}{2} \left[ k_w(\psi^{t+\Delta t}_{p1}) + k_w(\psi^{t+\Delta t}_{p2}) \right] \right\} - 
\frac{L}{12} \left\{ \left( 1 - \theta \right) m^w_2 (\psi^t_{p1}) + \theta m^w_2 (\psi^{t+\Delta t}_{p1}) \right\} + 
\frac{L}{12} \left\{ \left( 1 - \theta \right) m^w_2 (\psi^t_{p2}) + \theta m^w_2 (\psi^{t+\Delta t}_{p2}) \right\} \tag{27}
\]
The element $K_{21}$ can be expressed by:

$$K_{21} = -\frac{\Delta t}{\gamma_w L} \left\{ \frac{1}{2} \left[ k_w(\psi_{p1}^{t+\Delta t}) + k_w(\psi_{p2}^{t+\Delta t}) \right] \right\} - \frac{L}{12} \left\{ \left[ (1 - \theta) m_{2}^{w}(\psi_{p1}^{t}) + \theta m_{2}^{w}(\psi_{p1}^{t+\Delta t}) \right] + \left[ (1 - \theta) m_{2}^{w}(\psi_{p2}^{t}) + \theta m_{2}^{w}(\psi_{p2}^{t+\Delta t}) \right] \right\}$$

(28)

The element $K_{22}$ can be expressed by:

$$K_{22} = \frac{\Delta t}{\gamma_w L} \left\{ \frac{1}{2} \left[ k_w(\psi_{p1}^{t+\Delta t}) + k_w(\psi_{p2}^{t+\Delta t}) \right] \right\} - \frac{L}{2} \left\{ \left( 2 - \sqrt{3} \right) \left[ (1 - \theta) m_{2}^{w}(\psi_{p1}^{t}) + \theta m_{2}^{w}(\psi_{p1}^{t+\Delta t}) \right] + \left( 2 + \sqrt{3} \right) \left[ (1 - \theta) m_{2}^{w}(\psi_{p2}^{t}) + \theta m_{2}^{w}(\psi_{p2}^{t+\Delta t}) \right] \right\}$$

(29)

The element $B_{1}$ of the vector $\{B\}$ can be represented by:

$$B_{1} = -\frac{L}{2} \left\{ \left( 1 + \frac{1}{\sqrt{3}} \right) \psi_{p1}^{t} \left[ (1 - \theta) m_{2}^{w}(\psi_{p1}^{t}) + \theta m_{2}^{w}(\psi_{p1}^{t+\Delta t}) \right] + \left( 1 - \frac{1}{\sqrt{3}} \right) \psi_{p2}^{t} \left[ (1 - \theta) m_{2}^{w}(\psi_{p2}^{t}) + \theta m_{2}^{w}(\psi_{p2}^{t+\Delta t}) \right] \right\} - \frac{\Delta t}{\gamma_w L} \left( \psi_{2}^{t} - \psi_{1}^{t} \right) \left\{ \left( 1 - \theta \right) k_w(\psi_{p1}^{t}) + k_w(\psi_{p2}^{t}) \right\} - \Delta t \left[ (1 - \theta) q_{w}^{t} + \theta q_{w}^{t+\Delta t} \right] - \frac{\Delta t}{2} \left[ k_w(\psi_{p1}^{t+\Delta t}) + k_w(\psi_{p2}^{t+\Delta t}) \right]$$

(30)

The element $B_{2}$ of the vector $\{B\}$ can be represented by:

$$B_{2} = -\frac{L}{2} \left\{ \left( 1 - \frac{1}{\sqrt{3}} \right) \psi_{p1}^{t} \left[ (1 - \theta) m_{2}^{w}(\psi_{p1}^{t}) + \theta m_{2}^{w}(\psi_{p1}^{t+\Delta t}) \right] + \left( 1 + \frac{1}{\sqrt{3}} \right) \psi_{p2}^{t} \left[ (1 - \theta) m_{2}^{w}(\psi_{p2}^{t}) + \theta m_{2}^{w}(\psi_{p2}^{t+\Delta t}) \right] \right\} - \frac{\Delta t}{\gamma_w L} \left( \psi_{2}^{t} - \psi_{1}^{t} \right) \left\{ \left( 1 - \theta \right) k_w(\psi_{p1}^{t}) + k_w(\psi_{p2}^{t}) \right\} + \Delta t \left[ (1 - \theta) q_{w}^{t} + \theta q_{w}^{t+\Delta t} \right] + \frac{\Delta t}{2} \left[ k_w(\psi_{p1}^{t+\Delta t}) + k_w(\psi_{p2}^{t+\Delta t}) \right]$$

(31)

Finally, the solution is achieved by solving the global equation system:

$$[K]\{\psi^{t+\Delta t}\} = \{B\}$$

(32)

4. Concluding Remarks

Based on the Richard’s equation, a finite element to solve the nonlinear equation of flux in unsaturated porous media is proposed in this work. Through the water retention curve and the
coefficient of permeability of the geomaterials, problems in unsaturated media can be solved by the methodology herein presented.

The 1-D finite element proposed in this work can be easily extended to bi- or tridimensional solutions just by considering the variation of the parameters in these degrees of freedom. However, like any other numerical solution, dimensionality reduction must be considered prior to the implementation in order to achieve better performance of the code and to avoid needless iteration, since the consideration of unsaturated flux already requires greater computational effort than the saturated one.

Future works will address the remarkable characteristics of stability and convergence of this formulation. Due to these characteristics, as Richards’ equation is nonlinear, the iterative method for solving it should be simple recalculation of $m_{2,w,t+\Delta t}$ and $k_{w,t+\Delta t}$, followed by re-solving the linear system, until any convergence criterion for $\psi^{t+\Delta t}$ is attained.

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