

# Numerical study of non-saturated porous media flow

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Abstract. Water is an essential natural resource in maintenance of life, considering physiological/biochemical aspects related to living beings. In addition, water is livelihood for plants and animal species. Water resources play an important role in countries' economic development, as industries demand large volumes of water to manufacture products. In agriculture, water is widely used for crop production, guaranteeing the supply of food to the population. Due to the large use of such natural resource, it is necessary the optimization of its use. Irrigation systems are required to supply the necessary amount of water to the soil, providing ideal humidity for plant growth. Prediction of retention curve is an essential tool to describe water flow in soils, providing an estimative of water availability used in plant growth, at different depths. The present work aims to study the water retention curve of the non-saturated flow problem in soils by performing a numerical simulation of the soil moisture profile with reported data in the literature, using Picard iterative scheme. To prove the effectiveness of the method, a comparison with an implicit scheme is made, both based on finite differences.

Keywords: Richards' equation, Mathematical modelling, Soil science, Retention curve

## 1 Introduction

List and Radu [1] reported several relevant applications related to non-saturated porous media flow phenomena in Soil Science, such as water profiles description and bioremediation, a process used to threat contaminated media, includind water and oil. Numerical simulations are useful to solve and understand the dynamics of such problems. Associated modelling usually involves solving nonlinear partial differential equations, affiliated to nonlinear parameters.

According to Libardi [2], the study of water flow in soils under isothermal conditions began in 1856, with the contribution of the hydraulic engineer Henry Darcy. Darcy's equation describes the dynamics of water under saturation conditions. Later, in 1907, Buckingham mathematically described the movement of water in both saturated and unsaturated soils. In 1931, Richards [3] used Continuity and Darcy-Buckingham equations, generating Richards' equation, which contributed strongly to the consolidation of the theory that represents the dynamics of water in soil-water-plant systems.

Despite its easy deduction, Richards' equation is a difficult nonlinear partial differential equation to be solved analytically using conventional techniques, as it depends on nonlinear parameters. Therefore, numerical methods are used to solve the problem (Farthing and Ogden [4]). Over the last decades, studies of Celia et al. [5] contributed to the advances in Soil Science, solving Richards' equation by making approximations applied to the spatial domain using finite elements and finite differences methods, coupled with one-step backward Euler method, in which nonlinear equations are generated, using modified Picard method as an iterative procedure for linearizing discretized equations. Richards' equation can be written in 3 different ways: h-based (pressure head),  $\theta$ -based (moisture content) and mixed forms. In this paper, the h-based form is adopted, using data from Celia et al. [5], which is mentioned by other authors, such as Farthing and Ogden [4], Caviedes-Voullieme et al. [6], Ogden and Lai [7], Zambra et al. [8], Bouchemella et al. [9], Shanmugam et al. [10] and Vasconcellos and Amorim [11], making discussions about stability, efficiency and convergence of solutions in different ways. A complete review of numerical solutions related to Richards' equation can be found in Farthing and Ogden [4].

Richards' equation depends on the water content in the soil, the hydraulic conductivity and the matric potential. Such parameters are highly non-linear, and it is necessary to find relationships between them to find a solution to the differential equation. Water retention curve keeps the relationship between water content and pressure head in unsaturated systems (Shanmugam et al. [10], Celia et al. [5]). Expressions for hydraulic conductivity are cited in the literature, as in the works of Haverkamp [12] and Van Genuchten [13], which analytically represent soil moisture, hydraulic conductivity and matric potential. This paper adopts the Haverkamp model.

This paper is intended to simulate the one-dimensional infiltration phenomena through unsaturated zone via Richards' equation using soil parameters reported by Haverkamp [12] in work of Celia et al. [5], resulting the soil water profile, seen as a relationship between pressure head (h) and depth (z). The difference finite approximation coupled with an one-step backward Euler time-marching was chosen. This was applied to a modified Picard scheme to linearize discretized equations. Results were compared to implicit scheme proposed for Celia et al. [5]. Residual analysis using different time steps were executed in order to validate the simulation. Finally, the retention curve of the implicit scheme was made, considering  $\Delta t = 1$  sec.

#### 2 Mathematical approach

The h-based form of Richards' equation is

$$C(h)\frac{\partial h}{\partial t} - \vec{\nabla} \cdot \left[ K(h)\vec{\nabla}h \right] - \frac{\partial K(h)}{\partial z} = 0, \tag{1}$$

where z is vertical coordinate, assumed positive upward [L], t is time [T], h is pressure head [L], K(h) is the unsaturated hydraulic conductivity function  $[LT^{-1}]$ ,  $C(h) = \partial \theta / \partial h$  is the specific moisture capacity function  $[L^{-1}]$ , where  $\theta$  is the moisture content  $[L^3L^{-3}]$ . Temporal discretization of eq. (1) using a backward Euler method may be written as

$$C^{n+1}\frac{H^{n+1} - H^n}{\Delta t} - \nabla K^{n+1}\nabla H^{n+1} - \frac{\partial K^{n+1}}{\partial z} = 0,$$
(2)

where  $H^n$  is the approximate value of h in the *n*-th discrete time level  $(t = t^n)$ ,  $\Delta t = t^{n+1} - t^n$  is the step time,  $C^{n+1}$  and  $K^{n+1}$  are evaluated using  $H^{n+1}$ , and the solution is known at time level n and unknown at n + 1. According to Celia et al. [5], spatial approximation may be written using Picard iterative scheme, which produces successive estimates of the unknown  $H^{n+1}$  from the last estimates of  $C^{n+1}$  and  $K^{n+1}$ , providing some linearization of the discretized equations. Considering m as the iteration level and constant spacing  $\Delta z$ , the onedimensional case of Richards' equation can be written as

$$C_{i}^{n+1,m}\frac{\delta_{i}^{m}}{\Delta t} - \frac{1}{(\Delta z)^{2}} \left[ K_{i+\frac{1}{2}}^{n+1,m}(\delta_{i+1}^{m} - \delta_{i}^{m}) - K_{i-\frac{1}{2}}^{n+1,m}(\delta_{i}^{m} - \delta_{i-1}^{m}) \right]$$
  
$$= \frac{1}{(\Delta z)^{2}} \left[ K_{i+\frac{1}{2}}^{n+1,m}(H_{i+1}^{n+1,m} - H_{i}^{n+1,m}) - K_{i-\frac{1}{2}}^{n+1,m}(H_{i}^{n+1,m} - H_{i-1}^{n+1,m}) \right]$$
  
$$+ \frac{K_{i+\frac{1}{2}}^{n+1,m} - K_{i-\frac{1}{2}}^{n+1,m}}{\Delta z} - C_{i}^{n+1,m} \frac{H_{i}^{n+1,m} - H_{i}^{n}}{\Delta t} = (R_{i}^{n+1,m})_{RDF},$$
(3)

where  $\delta_i^m = (H_i^{n+1,m+1} - H_i^{n+1,m})$  is the increment in the iteration. Residual  $(R_i^{n+1,m})_{RDF}$  is a measure of the error for the spatial approximation using finite difference method coupled to the Picard iterative scheme. In terms of convergence, both residual and the difference between each iteration approximate to zero. In addition,  $K_{i\pm\frac{1}{2}}$  is defined as the arithmetic average between  $K_i$  e  $K_{i\pm1}$ .

In order to solve Richards' equation, hydraulic conductivity models are required. In this paper, the model of Haverkamp [12] is adopted, which describes relationships between  $\theta \in K$  as functions of pressure head h, namely

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$$\theta(h) = \frac{\alpha \left(\theta_s - \theta_r\right)}{\alpha + \left|h\right|^{\beta}} + \theta_r \tag{4}$$

and

$$K(h) = K_s \frac{A}{A + |h|^{\gamma}},\tag{5}$$

where  $\alpha$ ,  $\beta$ ,  $\gamma$ , A are empirical constants,  $K_s[LT^{-1}]$  is the hydraulic conductivity of the saturated soil.

#### **3** Preliminary results

A numerical simulation of non-saturated porous media flow was carried out in this work, considering onedimensional case, where z [L] is the vertical coordinate, assumed positive upwards. The proposal is to solve the *h*-based form of Richards' equation, using finite differences method as a spatial approximation, discretizing the domain in 41 points. Also, the backward Euler method is coupled as a temporal approximation. Picard's iterative scheme was used to linearize the discretized equations. As a result, the pressure head values *h* [L] are obtained as a function of the depth *z* [L]. Data generated are applied in the Haverkamp hydraulic conductivity model in order to create the retention curve for the phenomenon. The code to implement this algorithm for numerical solution of eq. (1) was written in FORTRAN, using  $10^{-8}$  as a tolerance. In addition, the figures came from Octave.

Initial and boundary conditions as well as soil parameters are required to solve Richards' equation for unidimensional flow in unsaturated soil. Considering the problem reported by Haverkamp [12],  $\alpha = 1, 611.10^6$ ,  $\theta_s = 0, 287, \theta_r = 0,075, \beta = 3,96, K_s = 0,00944$  cm/s,  $A = 1,175.10^6$  and  $\gamma = 4,74$ . In addition, considering a 40 cm soil column depth, with inicial condition h(z,0) = -61,5 cm, boundary conditions  $h(40,t) = h_{top} = -20,7$  cm and  $h(0,t) = h_{bottom} = -61,5$  cm, the solution was simulated in time elapsed for 360 seconds, and generated for different time steps  $\Delta t$ , with  $\Delta z = 1$  cm. The results were compared with Celia et al. [5].



Figure 1. Comparison of results with CELIA et al.[5]

Analyzing the obtained results in Fig. 1, the simulation was able to accurately capture the water profile points generated by Celia and coworkers, which demonstrates its feasibility of describing the movement of water in unsaturated soils. In order to evaluate the behavior of the error considering different  $\Delta t$  values, a graph expressing the relationship between the residue and the number of iterations for the first time step is required.



Figure 2. Semilog graph, expressing the behavior of the residual

According to Figs. 1 and 2, it is clear to see that the solutions are convergent in different  $\Delta t$  values, however the results are noticeably underestimated for  $\Delta t$  values bigger than 10 seconds. This was reported by Celia et al [5]. Also, in both cases the residual decreases with the number of iterations, but considering big  $\Delta t$  values the number of iterations required increases, demanding additional computational efforts. In such cases, residuals has an oscilatory, decreasing behavior. Using obtained data with  $\Delta t = 1.0$  sec., it was possible to generate the retention curve associated with the phenomenon, which describes the soil moisture values  $\theta [L^3 L^{-3}]$  as a function of the pressure head h [L].



Figure 3. Retention curve.

Above, Fig. 3 is obtained using Haverkamp [12] model, which is crucial to predict water content in soil, as this describes how, when a soil is dried from saturation, the moisture content decreases as the pressure head becomes more negative.

#### 4 Conclusions

Based in this paper, the simulation of one-dimensional infiltration phenomena proved to be effective in describing water movement through unsaturated zone. Water profiles were successfully generated considering different  $\Delta t$  values. Residuals that came from finite differences approximation coupled with a backward Euler method, associated to Picard iterative scheme behaved reasonably well if step time is not too big, which is in agreement with Celia and coworkers. The aim of this paper was reached, which is the prediction of retention curve associated to the phenomena, keeping a relationship between moisture content and pressure head. Prediction of retention curve is important in agriculture, as use of water may be optimized.

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