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Numerical Modeling of Underground Flow Through Porous Media Using a Finite Volumes Scheme

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ABSTRACT: The Richards equation attracts the attention of several researchers due to its importance in the hydrogeology field especially the flow through porous soil. It is a non linear partial differential equation that has no general analytic solution. Thus, the need to use numerical methods to solve it. In this work, a finite volumes scheme is used to simulate the pressure form and the mixed form of Richards equation in one dimension. Euler explicit and implicit schemes are used for the time discretization and a condition of scheme's stability is given. Different test cases are done to validate the accuracy and the efficiency of the proposed numerical model.

Key Words: Finite volumes method, Richards equation, porous media.

Contents

1. Introduction

The flow through porous soil is a complicated phenomena that has been the main subject of many studies in applied mathematics and hydrology in recent decades. The most famous model dealing with this topic is the one introduced by Richards [31]. The Richards equation describes flow in a variably saturated porous soil. It is a parabolic equation that has no general analytical solution. In this paper, we analyze three forms of this equation to study the behavior of the differential equations and the numerical methods used.

Comprehensive colloid transport in porous media under transient-flow conditions is pivotal in conception contaminant transport in soil or the vadose zone where flow conditions vary ever (see Fig. 1). To date, miscellaneous decades of research have been dedicated to improve understanding of the fate and transport of colloids in porous media (see, [5,26]). It has been instituted that colloid transport and retention in porous media are mostly steward by advection, dispersion, and inactivation, as well as by colloid

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interactions with several interfaces (see, [22,33]). Based on years of research, it is extensively admitted that due to their small size, colloidal suspensions rolling quickly porous media are expelled from pores sharply which they physically cannot fit, they have limited diffusivity (see, [20,35,44]), and are generally electrostatically repulsed from like-charged porous media surfaces (see, [30,39]). Research has also on view that depending on the flow regime and water glad of the porous media, the prevalent processes inspecting colloid transport, intercourse, retention, and remobilization can vary greatly influencing the appearance time, peak concentration, and leave distance of colloids transported in porous media (see, [9]). It is likewise understood that solution chemistry inclusive pH (see, [29]), ionic potency (see, [19]), and natural matter (see, [42]) as well as the framework and soil bead surface ruggedness (see, [30]) extend or hamper these processes.

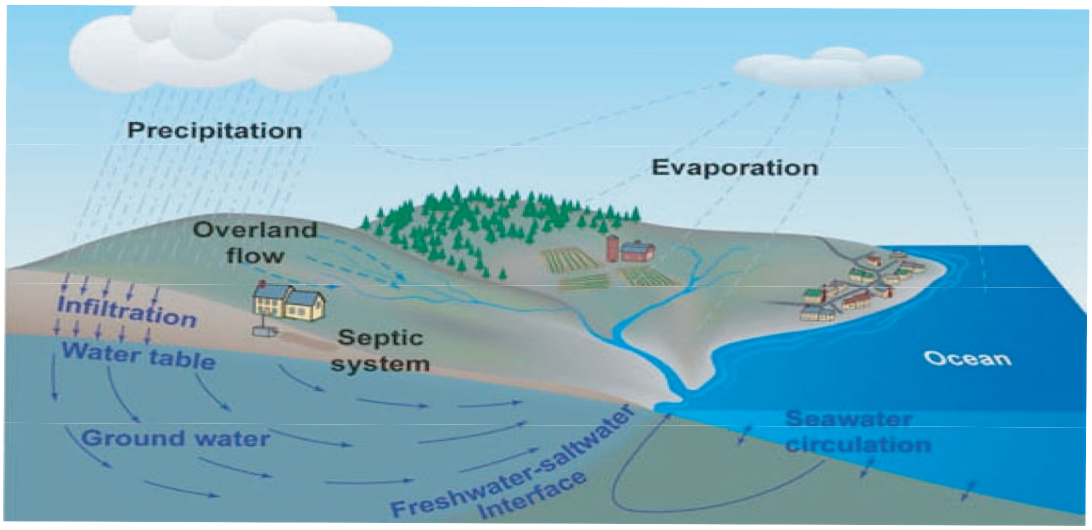

Figure 1: Schematic chart of flow through porous soil transfer processes

In the recent years, three numerical methods have been used to solve the Richards equation in its different forms:

- The finite differences method used by Celia and al. [10], and L. Fengnan et al. [16], F. Yasuhide et al. [43], Chávez–Negrete et al. [12] and references therein. Despite of the simplicity of this method, it does not take in consideration the discontinuity of the solution.
- The finite elements method (FEM) used by Forsyth and al. [17] and Pop et al. [27] and references therein. In this method more mathematics are involved but it has less physical significance. This method requires a resolution of a system of equations, which can causes some problems if is large.
- The finite volumes method (FVM) used by Eymard and al. [15], Pour et al. [28] and references therein.

In the literature, the finite elements method is widely used due to the nature of Richards equation, as the equation remains parabolic before saturation and becomes elliptic once the domain is fully saturated [18]. That being said, for its natural ability to ensure the mass conservation and taking account the discontinuity of the solution without solving any system, the finite volumes method is more used in recent years [25,32,36,37]. Thus, it is a very interesting and promising new approach.

The main goal of this paper is to develop and verify a Finite volumes based on one dimensional (1D) test cases. This work is motivated by the need to fully understand the numerical choices and their consequences to be able to build an efficient multidimensional solvers. Our study focuses on different aspects of a finite volumes scheme, the mass conservation, the stability, the accuracy, the efficiency, the continuity from the unsaturated to saturated regime (variable saturation) and the non-linearity of hydraulic conductivity and hydraulic capacity and its interaction with the finite volume method. In order to have a numerical model that simulates a single phase water flow through heterogenous soil. Four FVM models: Explicit/Implicit pressure forms, Explicit/Implicit mixed forms are derived by integrating the Richards equation, the Mualem-van Genuchten [41] and Brooks-Corey [8] soil model forward and backward Euler methods for time integration. A linearized stability analysis of two of the models completes the numerical discussion. In order to test the performance of these models, we use different Benchmark test cases for every single formulation.

The paper is organized in the following manner. In Section 2, we give the mathematical model and the governing equation. In Section 3, we propose a numerical model to solve Richards equation and we study the stability condition of the scheme. Finally, in section 4, we give several test cases for different forms of Richards equation.

2. Mathematical model and governing equation

Richards equation is extensively applied to model partially saturated fluid flow through porous media, such as soil. Parametrization of Richards' equation is stimulating, essentially for the reason that the difficulties in relating the parameters to facilely resolvable experimental values. The flow through the porous soil is described by Richards equation (Richards, 1931) which can be formulated as

$$\frac{\partial \theta(h,x,y,z)}{\partial t} = \nabla.[K(h,x,y,z)\nabla(h(x,y,z)+z)] + Q_s \tag{2.1}$$

where θ is the volumetric water content (water volume/total bulk volume), h is the pressure head, $K(h)$ is the hydraulic conductivity tensor and z is the vertical coordinate. We note here that the equation (2.1) is the mixed form of Richards equation, as it includes both θ and h explicitly. This form is associated to diffusion transport due to capillarity and advective transport resulting from gravity.

The Richards equation can be also written in pressure form, by introducing the definition of the hydraulic capacity $C(h) = \frac{\partial \theta}{\partial h}$

$$C(h)\frac{\partial h(x,y,z)}{\partial t} = \nabla.[K(h,x,y,z)\nabla(h(x,y,z)+z)] + Q_s \tag{2.2}$$

The Richards equation can be written also in water content form

$$\frac{\partial \theta}{\partial t} = \nabla.[D(\theta)\nabla\theta] + \nabla K(\theta) + Q_s \tag{2.3}$$

Where D is the diffusivity given by

$$D = K\frac{\partial h}{\partial \theta}.$$

The water content form is written in conservation form but it is impossible to solve the saturated case and discontinuities will arise for a heterogenous soil, while the pressure form gives a continuous results for heterogenous conditions and for both saturated and unsaturated media especially for the transition from. In the other hand, the mixed form has the advantages of both the other forms and guarantees conservation, continuity and the saturated/unsaturated conditions. Existence, uniqueness, and regularity of solutions of the problem (2.1) are studied for different boundary conditions by several authors (see [1,21,23,38,40], for instance).

2.1. Soil's empirical model

To define the different functions determining the Richards equation, several empirical models have been developed, in particular two are the well known in the literature due to their consistency. There are the Brooks-Corey (1964) model and the van Genuchten (1980).

2.1.1. Brooks-Corey model. The Brooks-Corey model [8] is expressed by

$$\begin{aligned} K(h) &= K_s[\tfrac{\theta_h-\theta_r}{\theta_s-\theta_r}]^{3+2/n}, \text{ if } h < h_d \\ &= K_s, \text{ elsewhere}, \end{aligned}$$

$$\begin{aligned} C(h) &= n\tfrac{\theta_s-\theta_r}{|h_d|}(\tfrac{h_d}{h})^{n+1}, \text{ if } h < h_d \\ &= 0, \text{ if } h \geq h_d, \end{aligned}$$

$$\begin{aligned} \theta(h) &= \theta_r + (\theta_s - \theta_r)\tfrac{h_d}{h}, \text{ if } h < h_d \\ &= \theta_s, \text{ if } h \geq h_d, \end{aligned}$$

where K_s is the saturated hydraulic conductivity, h_d the air inlet pressure is equal to the pressure capable of desaturating the pore wide in the field, θr is the residual water content, θs is the saturated water content, $n = 1 - 1/m$ and m parameters linked to the soil structure.

2.1.2. Van Genuchten model. In the Van Genuchten model [41], the hydraulic capacity $C(h)$, the hydraulic conductivity tensor $K(h)$ and the volumetric water content θ are expressed by

$$\begin{aligned} C(h) &= \tfrac{n*m*a\ |h|\ d\theta}{(1+(a*|h|)^n)^{1+m}}, \text{ if } h < 0 \\ &= S^*, \text{ if } h \geq 0, \end{aligned}$$

$$S_e = \frac{1}{(1 + a^n\,|h|^n)^m}$$

$$\begin{aligned} K(h) &= K_s\sqrt{S_e}(1 - \sqrt{1 - S_e^{\frac{1}{m}}})^m, \text{ if } h < 0 \\ &= K_s, \text{ if } h \geq 0, \end{aligned}$$

$$\begin{aligned} \theta(h) &= \theta_r + \tfrac{d\theta}{(1+(a*|h|))^n)^m}, \text{ if } h < 0 \\ &= \theta_s, \text{ if } h \geq 0, \end{aligned}$$

where K_s is the saturated hydraulic conductivity, $d\theta = \theta_s - \theta_r$ with θ_r is the residual water content, θ_s is the saturated water content, S^* is the specific volumetric storage capacity, $n = 1 - 1/m$ and m parameters linked to the soil structure. Note that in the unsaturated conditions we have $S_e = \frac{\theta-\theta_r}{\theta_s-\theta_r}$ and $S_e = 1$ for the saturated conditions.

3. Numerical model

In this section, we introduce several schemes to solve the pressure form and the mixed form for 1D flow. Results will presented to show the numerical consequences of each choice and their computational cost. The water content form is not developed here since it does not apply for the saturated conditions.

3.1. Spatial discretization

The Richards equation in its mixed form is first integrated over a control volume Ω, hence

$$\int_\Omega \frac{\partial\theta}{\partial t}d\Omega - \int_\Omega \nabla.\left(K\nabla(h+z)\right)d\Omega = \int_\Omega f d\Omega \tag{3.1}$$

Dependence of K and θ on h has been dropped in notation for simplicity but it should be remembered that such dependence still exists. Applying Green-Ostrogradski's theorem, the equation becomes

$$\frac{\partial\theta}{\partial t} \times \Omega - \int_S \left(K\nabla(h+z)\right).ndS = \Omega \times f_\Omega \tag{3.2}$$

where n is the outer-pointing normal vector of the control volume surface S. Finally, if the control volume Ω is discretized into finite volumes Ω_i and the surface S is discretized into N faces, each one is of length l, the finite volume scheme is written as follows

$$\frac{\partial \theta_i}{\partial t} \times \Omega_i - \sum_l \int_l K\nabla(h+z).n_l dx = \Omega_i \times f_{\Omega_i} \tag{3.3}$$

and then we obtain

$$\frac{\partial \theta_i}{\partial t} \times \Omega_i - \sum_l K_l \nabla_l (h+z).n_l.l = \Omega_i \times f_{\Omega_i} \tag{3.4}$$

Following the same steps on the pressure form of Richards equation, we obtain the finite volumes scheme

$$C_i \frac{\partial h}{\partial t} \times \Omega_i - \sum_l K_l \nabla_l (h+z).n_l.l = \Omega_i \times f_{\Omega_i} \tag{3.5}$$

The 1D simplification of Equation (3.5) with z pointing upwards, and $i = 0$ at the bottom of a column is written as

$$\frac{\partial \theta_i}{\partial t} = \frac{1}{\Delta z} \times (\phi_{i+1/2} - \phi_{i-1/2}) \tag{3.6}$$

where $K(h_{i+1/2}) = K_{i+1/2}$ and ϕ is a numerical flux chosen as

$$\phi_{i+1/2} = K_{i+1/2} \times (\frac{h_{i+1} - h_i}{\Delta z} + 1) \tag{3.7}$$

The equivalent of this scheme based on the pressure form as in Equation 3.4 leads to

$$C_i \frac{\partial h_i}{\partial t} = \frac{1}{\Delta z} \times (\phi_{i+1/2} - \phi_{i-1/2}) \tag{3.8}$$

where we use the same numerical flux as (3.7). The proposed method is second order accurate in space (see [11], for instance).

3.2. Time discretization

For the time discretization, the explicit and implicit Euler schemes are chosen for head and mixed formulations. Considering the pressure form of Richards equation and taking $C(h_i^n) = C_j^n$, the Euler explicit scheme is expressed by

$$C(h)\frac{\partial h(x,y,z)}{\partial t} = C_j^n \frac{h_i^{n+1} - h_i^n}{dt} \tag{3.9}$$

The Euler implicit scheme is given by

$$C(h)\frac{\partial h(x,y,z)}{\partial t} = C_j^{n-1} \frac{h_i^n - h_i^{n-1}}{dt} \tag{3.10}$$

For the mixed form of Richards equation, the Euler explicit scheme is expressed by

$$\frac{\partial \theta(h,x,y,z)}{\partial t} = \frac{\theta_i^{n+1} - \theta_i^n}{dt} \tag{3.11}$$

where $\theta(h) = \theta_i^n$. The Euler implicit scheme is written as

$$\frac{\partial \theta(h,x,y,z)}{\partial t} = \frac{\theta_i^n - \theta_i^{n-1}}{dt} \tag{3.12}$$

In conclusion, the finite volumes scheme of Richards equation mixed form 2.1 fully descritized for the explicit case as follows

$$\theta_i^{n+1} = \theta_i^n + \frac{\Delta t}{\Delta z \times C(h_i^n)} \times (\phi_{i+1/2}^n - \phi_{i-1/2}^n). \tag{3.13}$$

For the implicit case

$$\theta_i^n = \theta_i^{n-1} + \frac{\Delta t}{\Delta z \times C(h_i^n)} \times (\phi_{i+1/2}^n - \phi_{i-1/2}^n) \tag{3.14}$$

where $\phi_{i+1/2}^n = K_{i+1/2}^n \times (\frac{h_{i+1}^n - h_i^n}{\Delta z} + 1)$

The finite volumes scheme of Richards equation pressure form (2.2) is expressed for the explicit case as follows

$$h_i^{n+1} = h_i^n + \frac{\Delta t}{\Delta z \times C(h_i^n)} \times (\phi_{i+1/2}^n - \phi_{i-1/2}^n) \tag{3.15}$$

and for the implicit case:

$$h_i^n = h_i^{n-1} + \frac{\Delta t}{\Delta z \times C(h_i^n)} \times (\phi_{i+1/2}^n - \phi_{i-1/2}^n) \tag{3.16}$$

3.3. The stability of the scheme

The implicit scheme is unconditionally stable. For the explicit scheme, we set $H = h - z$, so the Richard's equation (2.2) becomes

$$C(h)\frac{\partial H}{\partial t} = \frac{\partial}{\partial z}\left[k(h)\left(\frac{\partial H}{\partial z}\right)\right] \tag{3.17}$$

The corresponding numerical scheme is written as follows

$$H_j^{n+1} = H_j^n + \frac{\Delta t}{\Delta z^2 C_j^n}[k_{j+\frac{1}{2}}^n (H_{j+1}^n - H_j^n) - k_{j-\frac{1}{2}}^n (H_j^n - H_{j-1}^n)] \tag{3.18}$$

If we take

$$\Delta H_{j+\frac{1}{2}}^n = H_{j+1}^n - H_j^n \tag{3.19}$$

and also

$$\Delta H_{j-\frac{1}{2}}^n = H_j^n - H_{j-1}^n \tag{3.20}$$

We obtain as a result

$$H_j^{n+1} = H_j^n + \frac{\Delta t}{\Delta z^2 C_j^n}[k_{j+\frac{1}{2}}^n \Delta H_{j+\frac{1}{2}}^n - k_{j-\frac{1}{2}}^n \Delta H_{j-\frac{1}{2}}^n] \tag{3.21}$$

by taking

$$C_{j+\frac{1}{2}}^n = \frac{\Delta t}{\Delta z^2 C_j^n} \times k_{j+\frac{1}{2}}^n \tag{3.22}$$

and

$$D_{j+\frac{1}{2}}^n = \frac{\Delta t}{\Delta z^2 C_j^n} \times k_{j-\frac{1}{2}}^n \tag{3.23}$$

this leads to

$$H_j^{n+1} = H_j^n + C_{j+\frac{1}{2}}^n \Delta H_{j+\frac{1}{2}}^n - D_{j-\frac{1}{2}}^n \Delta H_{j-\frac{1}{2}}^n \tag{3.24}$$

Thus, in order to guarantee stability, the following two conditions have to be satisfied

$$C_{j+\frac{1}{2}}^n + D_{j+\frac{1}{2}}^n \leq 1 \tag{3.25}$$

$$C_{j+\frac{1}{2}}^n + D_{j+\frac{1}{2}}^n \leq 1 \tag{3.26}$$

As a result, we get that

$$\frac{2\Delta t}{\Delta z^2 C_j^n} \times k_{j-\frac{1}{2}}^n \leq 1 \tag{3.27}$$

Furthermore, we know that

$$\frac{2\Delta t}{\Delta z^2 \times C_j^n} \times k_{j-\frac{1}{2}}^n \leq \frac{2\Delta t \times \max(K)}{\Delta z^2 \times \inf(C)} = CFL \tag{3.28}$$

In conclusion, the stability condition for our scheme is expressed as follows

$$\Delta t \leq CFL \times \frac{\inf(C) \times \Delta z^2}{2 \times \max(K)} \tag{3.29}$$

4. Numerical resultes

In this section, we present different test cases to illustrate our theoretical results of the model of the Richards equation in 1D expressed in its pressure formulation and its mixed formulation.

4.1. Test case 1:

In this subsection, the results are presented in the explicit 1D case for a homogeneous soil consisting of sand. The permeability K and water content θ as well as the hydraulic capacity C are defined according to the Van Genuchten model introduced below. The parameters taken for this test case are: saturated hydraulic conductivity $K_s = 6.26 \times 10^{-3}$, parameter $a = 0.028$, soil parameters $n = 1.3954$ and $m = 0.28$, saturated water content $\theta_s = 0.3658$ and residual water content $\theta_r = 0.0286$.

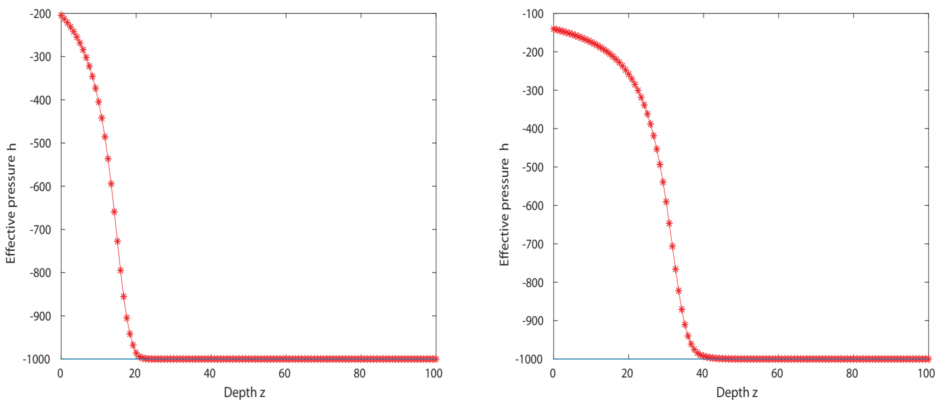

Figure 2: Head water in 12 hours (left) and 5 days (right)

For a number of points of $N = 200$ the infiltration is done rather quickly after 5 days and we notice that the homogeneity of the soil allows to have a rather smooth saturation, see Figure 2.

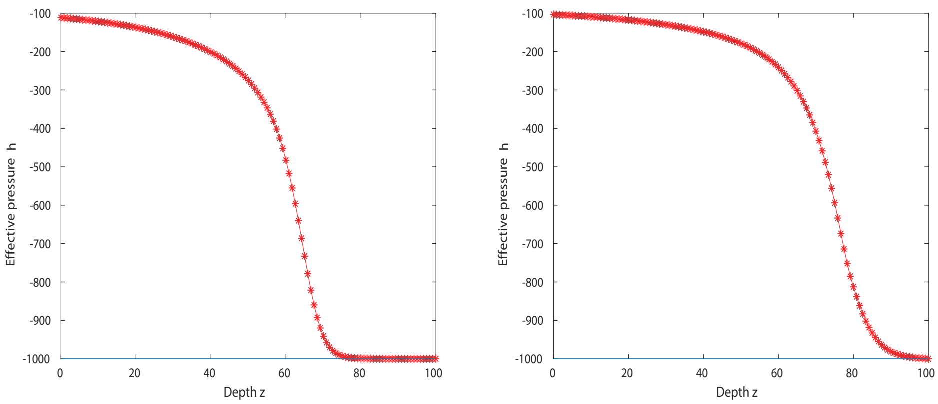

Figure 3: Head water in 14 days (left) and in 19 days (right)

The water continues to infiltrate the soil after 14 days, keeping a smooth shape of the water elevation. After 19 days, the soil is almost completely saturated, see Figure 3. One can see that the results are quite consistent with the physics of the problem.

4.2. Test case 2:

In this test case, we are interested in the coupling of the Richards equation in its pressure form and the transport equation. As in the previous test case, the hydraulic capacity C and and the hydraulic conductivity are expressed using the Van Genuchten formula. Thus, Richards equation is expressed in the same form

$$C(h)\frac{\partial h}{\partial t} = \frac{\partial}{\partial z}\left[K(h)\left(\frac{\partial h}{\partial z}+1\right)\right] \tag{4.1}$$

and we consider the transport equation in one dimension, taking into account a physical diffusive flow $\theta D \frac{\partial c}{\partial z}$, in the following form

$$\frac{\partial \theta c}{\partial t} + \frac{\partial qc}{\partial z} = \frac{\partial}{\partial z}\left(\theta D \frac{\partial c}{\partial z}\right) \tag{4.2}$$

The transport velocity is calculated based on Darcy's flow from Richards equation and it is expressed as

$$q = K(h)\left(\frac{\partial h}{\partial z}+1\right) \tag{4.3}$$

For this test case we consider the same soil parameters and we obtain the following results for an explicit finite volume scheme

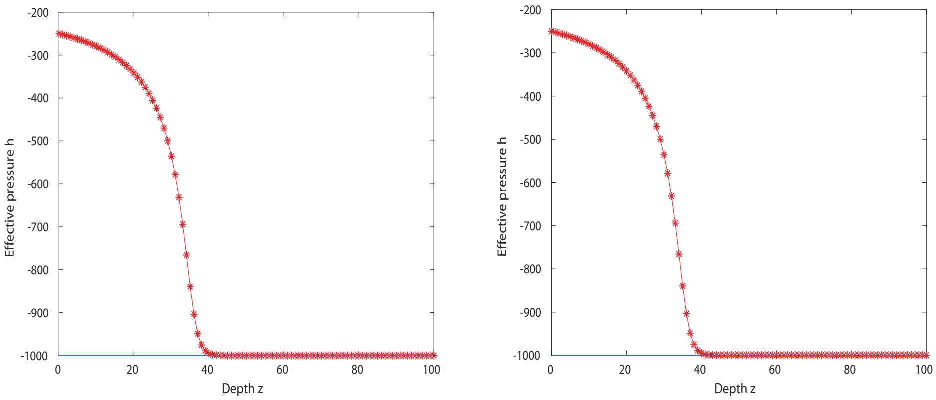

Figure 4: Water elevation water elevation in 9 day (left) and in 200 day (right)

One can see in Figure 4 and 5 that for a mesh of $N = 100$ we have relatively the same results of the previous test case and the soil becomes continuously saturated.

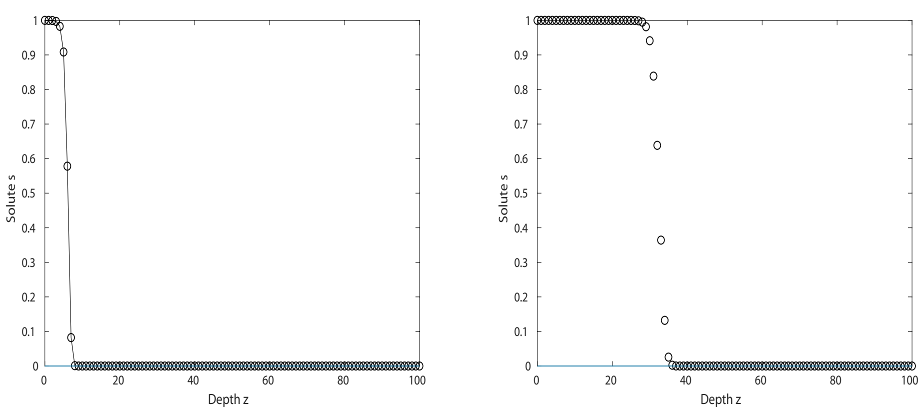

Figure 5: Concentration of the solute in 1 day (left) and in 5 days (right)

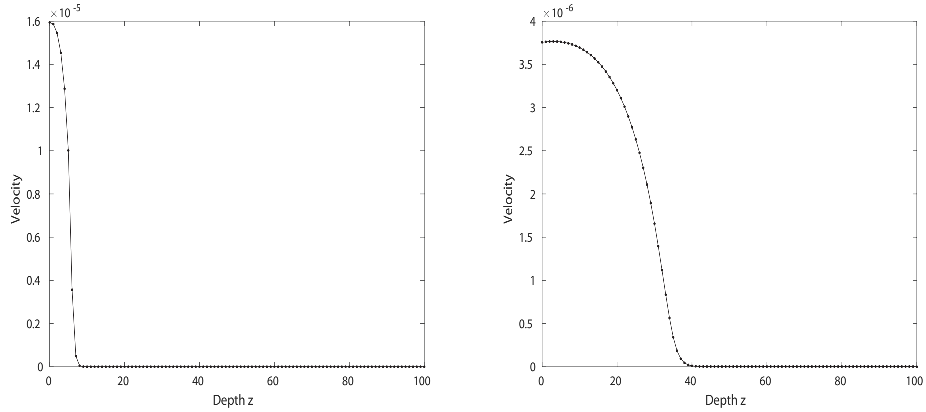

Figure 6: Transport velocity in 1 day (left) and in 5 days (right)

In Figure 6, it can be seen that the profiles of the transport velocity correspond relatively to the profiles of the water height, given that the velocity comes from the Darcy flow. The velocity follows well the infiltration pattern, which validates the coupling between the two equations.

4.3. Test case 3

In this test case, we validate our coupling model between the Richards equation and the transport equation for a heterogeneous soil. This remains an important difficulty with respect to the management of the transition zones between soil layers and given the strong non-linearity of the soil hydrodynamic parameters. We consider 5 layers consisting of sand and clay as shown in Figure 7.

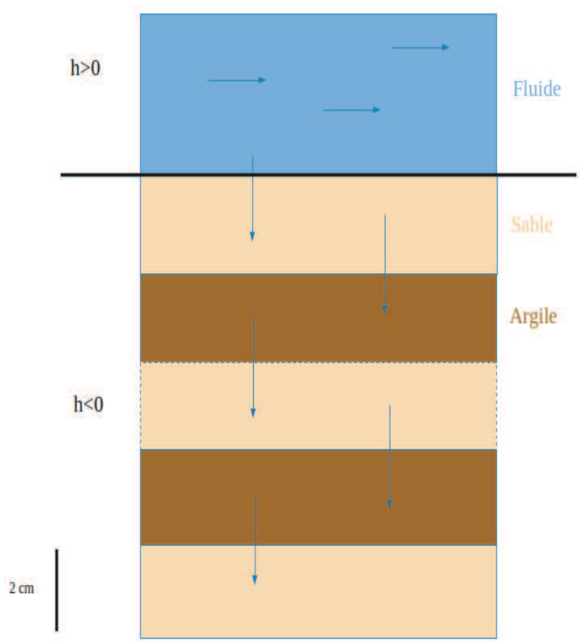

Figure 7: Soil constitution

The different physical parameters of the two soil types are summarized in the table below.

Soil	Parameters
Sand	$K_s = 0.00922\ cm/s$, $\theta_s = 0.368$, $\theta_r = 0.102$, $a = 0.0335\ cm^{-1}$
Clay	$K_s = 0.000151\ cm/s$, $\theta_s = 0.4686$, $\theta_r = 0.106$, $a = 0.03104\ cm^{-1}$

The numerical results of the coupling model for a domain of 100 *meters* and a number of points $N = 100$ are presented here using an explicit finite volume scheme.

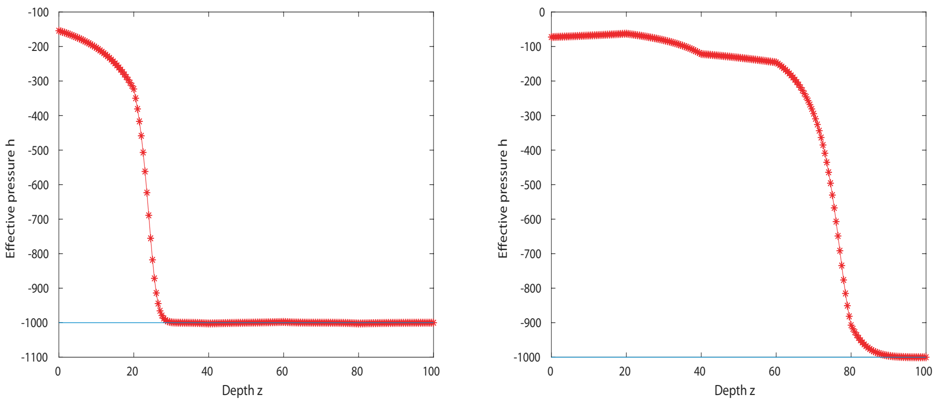

Figure 8: Water elevation in 5 days (left) and in 25 days (right)

The effect of soil heterogeneity on the water elevation profiles can be seen in Figure 8. This can be explained by the fact that the infiltration rate is no longer the same everywhere in the domain and differs according to the soil layers.

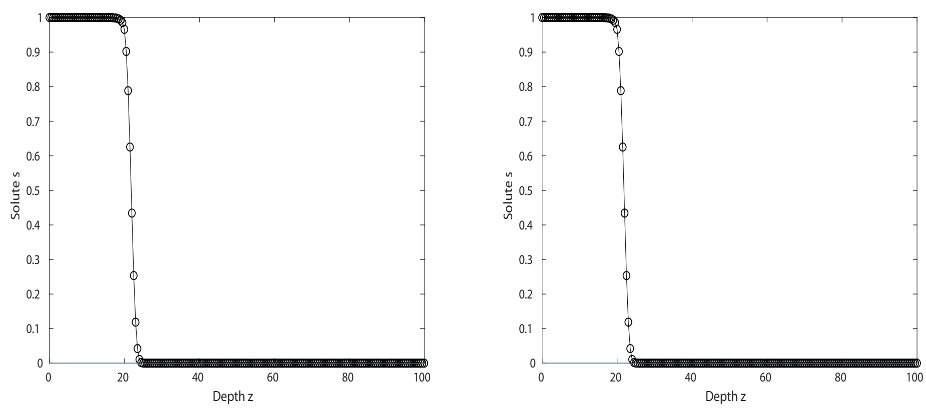

Figure 9: Solute concentration in 5 days (left) and in 25 days (right)

Figure 9 shows that the solute concentration profiles remain the same after 5 and 25 days. However, we note that the infiltration rate is no longer the same as that of homogeneous soil. This confirms that our model is able to capture the heterogeneity of the domain even for the transport part.

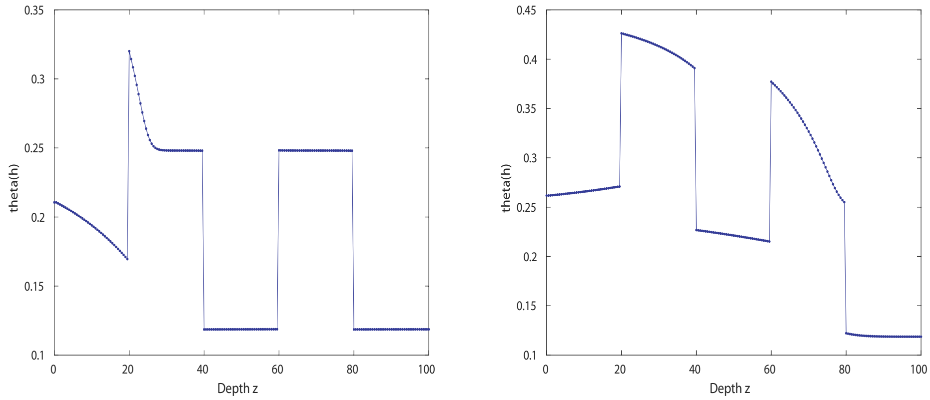

Figure 10: Water content in 5 days (left) and in 25 days (right)

Figure 10 shows more visibly the heterogeneity of the domain, which changes over time under the effect of soil saturation.

4.4. Test case 4

In this test case, we consider the Richards equation expressed in its mixed form. The hydrodynamic parameters K and θ will be expressed according to the Brooks model previously introduced. The following values are considered as soil parameters: $K_s = 0.00944$, $\theta_s = 0.287$, $\theta_r = 0.075$, $n = 3.96$ and $m = 4.74$. The initial solution is $h(z, t = 0) = -61.5\ cm$ and the boundary conditions $h(z = 0, t) = -61.5\ cm$ and $h(z = 40cm, t) = -20.7\ cm$. We present in Figures 11 and 12 the numerical results of our simulation using an implicit finite volume scheme.

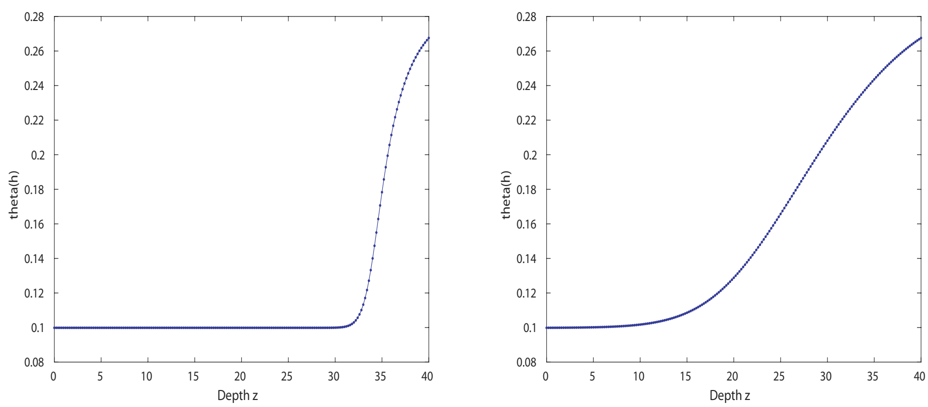

Figure 11: Water content in 5 days (left) and in 25 days (right)

Water content results show that the soil becomes saturated over time.

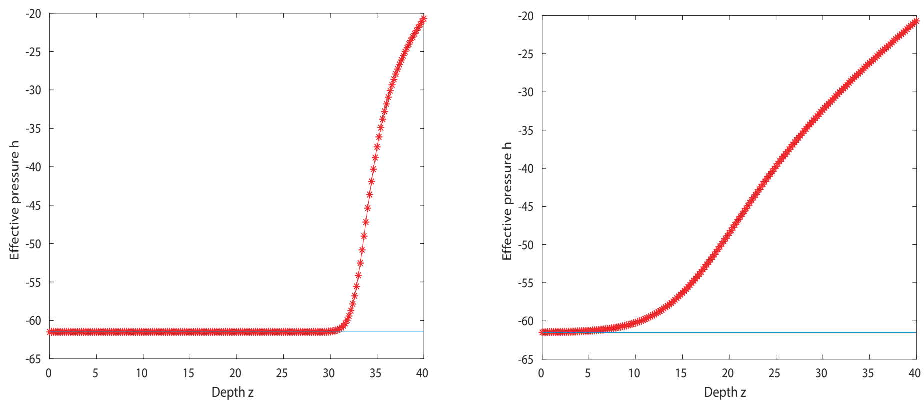

Figure 12: Water elevation h in 5 days (left) and in 25 days (right)

4.5. Test case 5:

In this test case, we consider the Van Genuchten model. In order to see the performance of our method, we implement it and the finite elements method. The parameters are taken as follows: saturated hydraulic conductivity $K_s = 8.78 \times 10^{-3}$, parameter $a = 0.0115$, soil parameters $n = 2.03$ and $m = 1 - \frac{1}{n}$, saturated water content $\theta_s = 0.52$ and residual water content $\theta_r = 0.218$. The numerical results of the coupling model for a domain of 100 *meters* and a number of points $N = 100$ are presented in Figure 13 using the cited methods. This figure shows that the obtained results by FVM agree with those given by EFM. Furthermore, for this example the computational time of FVM is 2.45 seconds, however for FEM is 9.05 seconds. This difference is justified by the higher computational cost needed to solve the system lying to EFM.

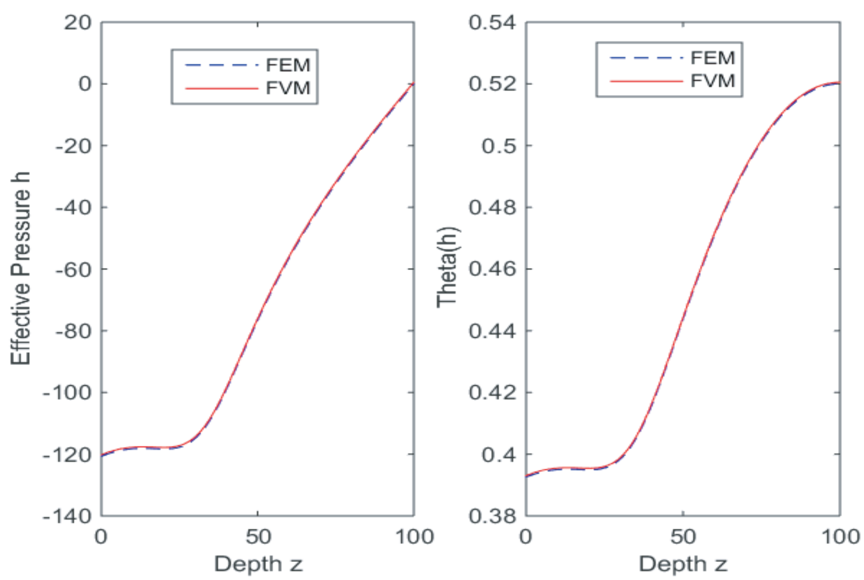

Figure 13: Water elevation (left) and Water content (right) in 45 minutes computed by FVM and FEM

5. Conclusion

In this work, we studied the numerical solution of Richards equation in its different forms using a finite volume scheme and an Euler time discretization. We studied four schemes based on the mixed form and the pressure form of Richards equation in the explicit and implicit time discretization. The explicit and implicit scheme based on the pressure form is accurate for homogenous and heterogenous soil for two soil models: Van Gunechten and Brooks-Corey. The mixed form of Richards equation results show accuracy and conservation for the explicit and implicit case. The explicit mixed scheme is conditionally stable and the stability constraints is similar to that of a diffusion equation. The implicit mixed scheme is shown to be unconditionally stable. The explicit scheme is severely less efficient because of stability constraints that do not allow large time steps, while the implicit scheme is able to generate accurate solutions with very large time steps.

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