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Kirchhoff Transformation of Richards Equation for Simulating Water Flow in Porous Media

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Abstract

A mathematical model that describes water flow through the unsaturated porous media is detailed in this paper. Indeed, this problem is based on the Richards equation. Resolution of such one-dimensional problem is performed using a Kirchhoff Transformation and a numerical approach based on the finite difference method.

Keywords

Porous Media, Water Flow, Kirchhoff Transformation, Finite Difference Method

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1. Introduction

In the next few years, groundwater contamination is the most important risk for water resources ([1]; [2]; [3]). The pollution process can be started by the discharge of industrial waste or pesticides and insecticides used in agriculture. Numerous studies were devoted to the prediction of solute transport migration through the unsaturated zone reaching groundwater ([4]; [5]; [6]; [7]). In arid and semi-arid regions, fresh waters contamination, in most cases, exceed the imposed values. It would be useful if modeling tools were available in order to allow the assessment of pollution and to develop relevant solutions [8]. A distinction can be made between models which rely on a deterministic approach, based primarily on the numerical resolution of the Richards equation for variably saturated flow, and the advection-dispersion equation for solute transport modeling [9]. These models are important tools for analyzing water and solute dynamics in the vadose zone. However, their use in the field remains limited ([10]; [11]) due to the large amount of critical data they require, such as hydrodynamic properties of the soil [12], solute transport parameters and climatic data. Risk assessment of pollution can be based on a quantitative approach, which requires understanding of the solute transport phenomena, from the water movement of the unsaturated soil zone to the aquifer [1].

Water flow in the vadose zone of unconsolidated and decompressed media is directed perpendicular to bedding; by contrast, groundwater flow mostly parallels bedding. This difference in flow orientation toward bedding expresses in a stronger transverse flow component and hydrodynamic dispersion ([13]; [14]) in the percolation zone than in aquifers [15]. Similar to groundwater flow in dual-porous media, there exists in the unsaturated zone a quick (preferential-flow) and slow flow (matrix-flow) component, which usually expresses in the unsaturated zone in greater differences of flow velocities than in aquifers; this is related to the fact that in the vadose zone hydraulic gradients can reach from close to zero till one and hydraulic conductivities may differ by several orders of magnitude; in general, this range of gradients and hydraulic conductivities is smaller in aquifers. As preferential-flow is not yet well quantifiable on the catchment scale and as the vadose zone is hydraulically more inhomogeneous than the groundwater zone, mathematical or numerical approaches on percolation are more difficult to achieve than on groundwater movement. According to climates and soil/sediment fabrics, matrix-flow in the unsaturated zone ranges from few meters to less than

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few millimeters per year. In humid areas, it is dominantly directed vertical down and in semi-arid to arid climates also vertical up according to the duration of drying and wetting cycles. In all climate zones, however, percolation can transform along beddings or ground-ice into inter-flow or perched groundwater, if high differences in the unsaturated hydraulic conductivities occur along these interfaces. Infiltration of precipitation generates in the vadose zone water storage, matrixand preferential-flow [16]; [17]; [18]; [19]; [20]). Preferential-flow interacts with matrix-flow by mass and ion exchange and often transforms partly or completely into inter-flow; it typically occurs in the upper part of the vadose zone of unconsolidated rocks and can by-pass the barrier function of soils for contaminants. In hydraulic models on percolation, the real range of porosities, unsaturated hydraulic conductivities, water contents, and water tensions in an REV can only be approached; therefore, the real system is generally characterized as a media with statistically equivalent properties. As a consequence, for the simulation of percolation and the determination of groundwater recharge, conceptual models suppose uni-directed fluxes, for example, vertical down and homogeneous equivalent hydraulic properties. This approach leads to compartment or box models [21], each with equivalents properties.

Typical parameters required for vadose zone numerical models are:

a) Bulk and particle densities,

b) The hydraulic conductivities from saturation till the residual water content,

c) Water contents and suctions at field capacity and at the wilting point,

d) Effective and total porosities for both saturated and unsaturated conditions,

e) Time series of water suctions and water contents at fixed places,

f) Climatologic data to determine evapo-transpiration,

g) Infiltration and overland-flow.

Contaminant behavior in the environment is complex and is governed by highly nonlinear processes. The phenomenon of groundwater contamination is the result of the instant combination of three processes: the water flow, the heat transfer and solute transport in the porous media [22]. It is recommended to study these processes and water movement separately. In this study, we propose a mathematical model for water flow simulation based on a Kirchhoff Transformation of Richards Equation [23].

2. Fundamentals of Richards Equation

The mass conservation is expressed by the continuity equation:

$$\frac{\partial \theta}{\partial t} = -\frac{\partial q}{\partial z} \tag{1}$$

where θ is the volumetric humidity, q is the flux and z is the depth. The Darcy law definition is:

$$q = -K\frac{\partial H}{\partial z} = K\left(1 - \frac{\partial h}{\partial z}\right) \tag{2}$$

where K is the hydraulic conductivity, H is the total head $(h - z)$ and h is the pressure head.

The mixed form of Richards equation [24] is given by the combination of equations (1) and (2):

$$\frac{\partial \theta}{\partial t} = -\frac{\partial}{\partial z}\left(K\left(1 - \frac{\partial h}{\partial z}\right)\right) \tag{3}$$

Equation (3) has two independent variables and does not have any stable numerical solutions.

If we define the capacity of soil humidity as $C = \frac{\partial \theta}{\partial h}$, we get:

$$C\frac{\partial h}{\partial t} = -\frac{\partial}{\partial z}\left(K\left(1 - \frac{\partial h}{\partial z}\right)\right) \tag{4}$$

According to [25] and [26] this form is more suitable for the saturated soil and has a programming problem for a Newton-Raphson algorithm.

Another form can be obtained by the definition of the soil diffusivity $D(\theta) = K(\theta)\frac{\partial \theta}{\partial h}$:

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}\left(D(\theta)\frac{\partial h}{\partial z}\right) - \frac{\partial K}{\partial \theta}.\frac{\partial \theta}{\partial z} \tag{5}$$

Equation (5) is widely used for modeling water flow in the unsaturated soils.

2.1. Kirchhoff Transformation of Richards Equation

In order to linearize equation (5) and to minimize spatial and temporal nonlinearities, we applied:

$$U=\int_{-\infty}^{h}K.dh=\int_{0}^{\theta}D.d\theta \tag{6}$$

The mixed form of Richards equation (3) become:

$$\frac{\partial\theta}{\partial t}=-\frac{\partial}{\partial z}\left(K\left(1-\frac{\partial U}{\partial z}\right)\right) \tag{7}$$

2.2. Numerical Resolution

This section describes the finite difference formulation adopted for the mass conservation equation and introduces the processing of the Kirchoff transformation to solve Richards equation.

A space-time grid $\left(z_i,t_j\right)$ is used and by selecting θ_i^j approximating θ at the time $t=j\Delta t$, we can approach the mass conservation equation using a Crank-Nicholson scheme. This implicit method has a second order accuracy in time and space, is stable and is hardly more complicated to use than the others more simple implicit methods.

Equations (1) become:

$$\frac{\theta_i^{j+1}-\theta_i^j}{\Delta t}=\frac{1}{2\Delta z}\left[\left(q_{i+1}^j-q_{i-1}^j\right)+\left(q_{i+1}^{j+1}-q_{i-1}^{j+1}\right)\right] \tag{8}$$

By reducing the space step by half and rearranging the terms, we get:

$$\left(\theta_i^{j+1}-\theta_i^j\right)\frac{\Delta z}{\Delta t}=q_{i+1/2}^j-q_{i-1/2}^j+q_{i+1/2}^{j+1}-q_{i-1/2}^{j+1} \tag{9}$$

Or more simply:

$$F_i=\left(q_{i+1/2}^j-q_{i-1/2}^j\right)+\left(q_{i+1/2}^{j+1}-q_{i-1/2}^{j+1}\right)+e_i \tag{10}$$

Where:

$$e_i=\left(\theta_i^{j+1}-\theta_i^j\right)\frac{\Delta z}{\Delta t}$$

$$q_{i+1/2}^j=K_{i+1/2}^j-\frac{U_{i+1}-U_i}{\Delta z}$$

$$\Delta z=(z_{i+1/2}-z_{i-1/2})=1/2(z_{i+1}-z_{i-1})$$

The Kirchhoff transformation of the mixed Richards equation is:

$$q=K-\frac{\partial U}{\partial z} \tag{11}$$

For the resolution scheme, we adopt a Newton-Raphson approach to achieve the convergence.

If we suppose that h is the primitive variable:

$$h_i^{n+1}=h_i^n-\frac{f\left(h_i^n\right)}{f'\left(h_i^n\right)} \tag{12}$$

Where $f\left(h_i^n\right)$ is continuously differentiable and represents the previous $F(h)$.

The three non-zero derivatives of the line i of the matrix are given by:

$$\begin{aligned}\frac{\partial F_i}{\partial h_{i-1}^{j+1}}&=\frac{\partial}{\partial h_{i-1}^{j+1}}\left(-q_{i-1/2}^{j+1}\right)\\ \frac{\partial F_i}{\partial h_i^{j+1}}&=\frac{\partial}{\partial h_i^{j+1}}\left(q_{i+1/2}^{j+1}-q_{i-1/2}^{j+1}+e_i\right).\\ \frac{\partial F_i}{\partial h_{i+1}^{j+1}}&=\frac{\partial}{\partial h_{i+1}^{j+1}}\left(q_{i+1/2}^{j+1}\right)\end{aligned} \tag{13}$$

We approach the intermediate derived points by a geometric mean:

$$\begin{aligned}K_{i-1/2}&=\sqrt{K_{i-1}.K_i}\\ \frac{\partial K_{i-1/2}}{\partial h_{i-1}}&=\frac{1}{2}\sqrt{\frac{K_i}{K_{i-1}}}\frac{\partial K_{i-1}}{\partial h_{i-1}}\\ \frac{\partial K_{i-1/2}}{\partial h_i}&=\frac{1}{2}\sqrt{\frac{K_{i-1}}{K_i}}\frac{\partial K_i}{\partial h_i}\\ \frac{\partial K_{i-1/2}}{\partial h_{i+1}}&=0\end{aligned} \tag{14}$$

We obtain from those relations, the final expressions:

$$\begin{aligned}\frac{\partial F_i}{\partial h_{i-1}^{j+1}}&=-\frac{1}{2}\sqrt{\frac{K_i^{j-1}}{K_{i-1}^{j+1}}}.\frac{\partial K_{i-1}^{j+1}}{\partial h_{i-1}^{j+1}}+\frac{K_{i-1}^{j+1}}{\Delta z}\\ \frac{\partial F_i}{\partial h_i^{j+1}}&=\frac{1}{2}\left[\sqrt{\frac{K_{i+1}^{j+1}}{K_i^{j+1}}}.\frac{\partial K_i^{j+1}}{\partial h_i^{j+1}}+\frac{K_i^{j+1}}{\Delta z}-\sqrt{\frac{K_{i+1}^{j+1}}{K_i^{j+1}}}.\frac{\partial K_{i-1}^{j+1}}{\partial h_i^{j+1}}+\frac{K_i^{j+1}}{\Delta z}\right]+\frac{\Delta z}{\Delta t}\frac{\partial\theta_i^{j+1}}{\partial h_i^{j+1}}\\ \frac{\partial F_i}{\partial h_{i+1}^{j+1}}&=\frac{1}{2}\sqrt{\frac{K_i^{j+1}}{K_{i+1}^{j+1}}}.\frac{\partial K_{i-1}^{j+1}}{\partial h_{i+1}^{j+1}}+\frac{K_{i+1}^{j+1}}{\Delta z}\end{aligned} \tag{15}$$

2.3. Boundary Conditions

Imposed pressure head at the upper boundary:

h_0 is known.

$F_0=0$ as h_0 is known.

Imposed flux at the upper boundary:

We suppose that $q_0>0$: $F_0=\left(q_{1/2}^j-q_0^j\right)+\left(q_{i1/2}^{j+1}-q_{i0}^{j+1}\right)+e_0$

Imposed flux at the lower boundary:

$$F_m=\left(q_m^j-q_{m-1/2}^j\right)+\left(q_m^{j+1}-q_{im-1/2}^{j+1}\right)+e_m$$

Gravity drainage:

Gravity drainage can be imposed either at the base node (in the case of a single-layer soil) or in an interface node separating two layers of soil (in the case of vertically heterogeneous soil). If we designated m as the node where gravity drainage occurs, then:

$$q_m = \beta.K_m(h_m) \text{ where } \beta = \frac{\partial h_m}{\partial z}$$

Infiltration Excess

Under the infiltration access conditions where the potential at the surface becomes positive, the infiltration flow is modified by:

$$q_0 = Infiltration - \frac{\partial h_0}{\Delta t} \text{ and then } \frac{\partial q}{\partial h} = -\frac{1}{\Delta t}$$

This modification is taken into account through its contribution to the surface flow.

3. Simulation

The simulation is carried out by Hydrus-1D model [27] in a loamy sandy soil with a typical saturation problem. The boundary condition is Dirichlet type with constant initial water content (0.1 cm^3 cm^{-3}). The used parameters are given in the following table.

Table 1. Input parameters in Hydrus-1D.

Depth (cm)	θr (cm^3 cm^{-3})	θs (cm^3 cm^{-3})	α (cm^{-1})	n (-)	K_s (cm d^{-1})
0-100	0.0543	0.1723	0.038421	1.6689	128

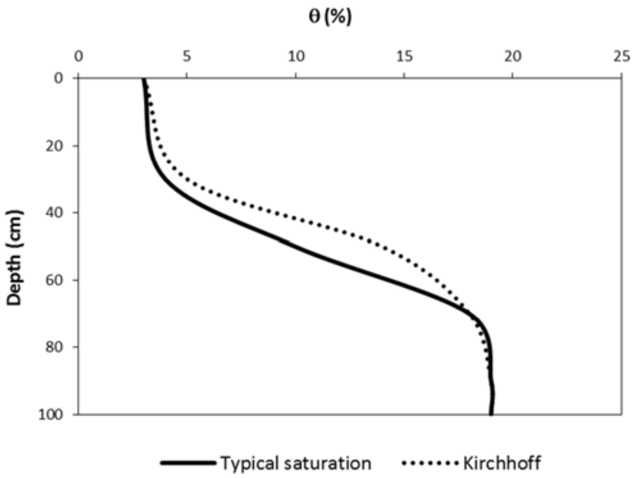

Figure 1. Water content variations.

The simulation result with Hydrus-1D was compared with the Kirchhoff's transformation model of the Richards equation as shown in figure 1. The same pattern of the soil water content is observed for the two models. However, the Kirchhoff's transformation model slightly overestimated the values around 50 cm in depth.

4. Conclusion

The numerical study that we conducted on water flow in homogeneous porous media shows that the Kirchhoff transformation of Richards Equation gives a strong and stable solution. The developed procedure does not involve unnecessary computation like that related to noise terms, which is a common problem for approximation methods like the homotopy perturbation method or others. This result allows us to combine the water flow model, based on the Richards equation, with solute transport equation to elaborate a more appropriate simulation of the contamination of groundwater through unsaturated soils.

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