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SIMULATING THE SATURATION FRONT USING A FRACTIONAL DIFFUSION MODEL

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Abstract. *In this paper the possibility of making use of fractional derivatives for the simulation of the flow of water through porous media and in particular through soils is considered. The Richards equation, which is a non-linear diffusion equation, will be taken as a basis and is used for the comparison of results. Fractional derivatives differ from derivatives of integer order in that they entail the whole history of the function in a weighted form and not only its local behavior, meaning that a different numerical approach is required. Previous work on the topic will be examined and a consistent approach based on fractional time evolutions will be presented.*

1 INTRODUCTION

Infiltration is defined as the flow of water through porous media and in particular through soils. It follows the ordinary laws of hydrodynamics. The Richards equation, which is a non-linear diffusion equation, is usually used for its description [1, 2, 3], even though in several cases it fails to predict variations in the behavior of different types of soil. The present work is an attempt to ascertain whether fractional calculus is suitable as a tool for the simulation of the saturation front in partially saturated porous media. Therefore the substitution of the derivative with respect to time with a fractional derivative of order smaller than unity is considered [4, 5]. Fractional calculus is a branch of mathematics related to integrals and derivatives of arbitrary order and dates back to the 17th century [6]. Fractional derivatives differ from derivatives of integer order in that they entail the whole history of the function in a weighted form and not only its local behavior. Lately it was found to have many applications in physics and mechanics, especially concerning the description of anomalous diffusion [7, 8]. It has been suggested[5] to replace the time derivative in the Richards equation by a fractional derivative as a way to describe experimental observations that show deviations from normal diffusive scaling. We found that the referenced paper [5] contains several theoretical errors (see also [9]), and we discuss ways how these can be eliminated. An improved and consistent approach based on fractional time evolutions [7] will be presented.

2 ABSORPTION IN POROUS MEDIA

2.1 Derivation of the Richards equation

A soil mass generally consists of a network of partially or totally interconnected interspaces of various sizes and shapes. These interspaces may be filled with air or water or both. The volumetric moisture content $\theta(t,\mathbf{x})$, also called local volume fraction of water, is defined as the ratio of the volume of water to the volume of a representative elementary soil volume located at position **x**. Under the assumption that the porosity (defined as the volume fraction of pores) is constant, and that the speed of the solid phase vanishes, the mass balance for the liquid phase yields:

$$\frac{\partial\theta}{\partial t} = -\mathrm{div}(\mathbf{q}) \qquad (1)$$

where $\mathbf{q}$ is the specific discharge of fluid through the interstices of the solid matrix. The flow of liquids in unsaturated media is determined by the pressure, gravity and capillary forces acting on the liquid. We consider the capillary potential (per unit weight of water):

$$\Psi = \left(p / \rho_w g + z \right) \tag{2}$$

where the pressure is determined by the surface tension and curvature of the air-liquid interface. We will consider horizontal absorption and therefore neglect the effect of gravity. Thus the moisture discharge vector is related to the total potential by means of the following equation:

$$\mathbf{q} = -K \cdot \mathrm{grad}\left(\Psi\right) \tag{3}$$

which is known as the moisture conduction equation. Combining equations (1) and (3) we acquire the following equation, known as the Richards equation:

$$\frac{\partial\theta}{\partial t} = \frac{\partial}{\partial x}\left(D(\theta)\frac{\partial}{\partial x}\theta\right) + \frac{\partial}{\partial y}\left(D(\theta)\frac{\partial}{\partial y}\theta\right) + \frac{\partial}{\partial z}\left(D(\theta)\frac{\partial}{\partial z}\theta\right) \tag{4}$$

where $D\left(\theta\right) = K\left(d\Psi / d\theta\right)$ is known as the moisture diffusivity. For example from Philip [10] we get the following empirical moisture diffusivity function

$$D \approx D_0 \exp(c \cdot \theta) \tag{5}$$

where $D_0 = 8.3 \cdot 10^{-7} cm^2 / min$ and $c = 19$. In Fig. 1 the experimental data and the fitted function of eq. (5) are presented. In what follows we will only consider one - dimensional moisture diffusion along horizontal soil columns. For this case the Richards equation will take the form

$$\frac{\partial\theta}{\partial t} = \frac{\partial}{\partial x}\left(D(\theta)\frac{\partial}{\partial x}\theta\right). \tag{6}$$

We choose the coordinate system such that $x = 0$ corresponds to the left end of the horizontal soil column.

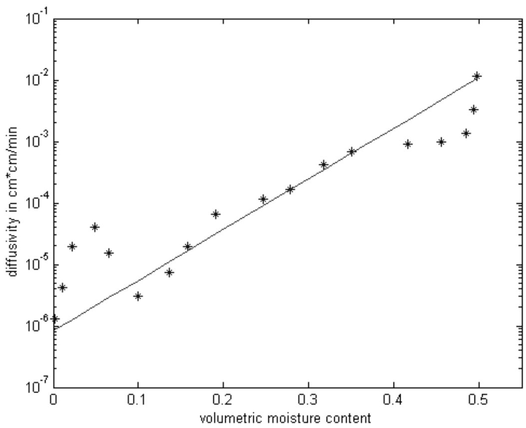

Fig. 1: Empirical diffusivity function from reference [10].
The fitted line corresponds to eq. (5).

2.2 Discussion

In the former analysis, the soil skeleton has been assumed to be rigid and the inertial effects have been assumed to be negligible, as the progress of the phenomenon is slow. The thermal effects and the effects of condensation and evaporation have been neglected, as well as the complications arising from the interplay of air and water [11,12]. With the introduction of the similarity variable

$$\xi = \frac{x}{\sqrt{t}} \tag{7}$$

Richard's equation (6) transforms into an ordinary differential equation, which has been used to find analytical solutions for soil water flow problems and also to find the dependence of the conductivity on the degree of saturation [13]. However, as summarized in a recent publication by Pachepsky et al. [5], significant deviations from the scaling law eq. (7) have been observed in many published experiments. Relationships between positions and times at which a particular value of the volumetric moisture content is observed suggest a similarity transformation of the form

$$\xi = x \cdot t^{-\alpha/2} \tag{8}$$

The case of $\alpha < 1$ could be interpreted as non-Brownian transport of particles that remain motionless for extended periods of time, for example, when waiting periods have a power law distribution.

In the aforementioned paper of Pachepsky et al. [5] the defect of Richards law is addressed by resorting into non-standard diffusion mathematical models that involve fractional derivatives with respect to time. It is worth noticing that one of us[4] has shown that the analysis of Pachepsky et al. (2003) et al. is mathematically flawed. An attempt to correct this analysis and the corresponding numerical integration of the fractional diffusion equation is shown below.

3 FRACTIONAL CALCULUS

Fractional calculus is the field of mathematical analysis which deals with the investigation and applications of integrals and derivatives of arbitrary order [6,7]. Although the term 'fractional calculus' is actually a misnomer, the designation 'integration and differentiation of arbitrary order' being more appropriate, it is well established due to prevailing use. In contrast to integration and differentiation of integer order, for integration and differentiation of arbitrary order a great variety of definitions exists. That is both one of the advantages and one of the disadvantages of fractional calculus.

If $f(x)$ is locally integrable on (γ,∞), then the right hand fractional Riemann-Liouville integral of $f(x)$ of order $\alpha > 0$ is defined as

$$I_{\gamma+}^{\alpha} f(x) = \frac{1}{\Gamma(\alpha)} \int_{\gamma}^{x} (x-u)^{\alpha-1} f(u) du \tag{9}$$

for almost all $-\infty < \gamma < x < \infty$ and for suitable f. The subscripts in I denote the terminals of integration in the given order.

The following general definition of fractional derivatives was introduced in [7]: The right sided fractional derivative of order $0 < \alpha < 1$ and type $0 \le \beta \le 1$ with respect to t is defined by

$$D_{\gamma+}^{\alpha,\beta} f(t) = \left(I_{\gamma+}^{\beta(1-\alpha)} \frac{d}{dt} \left(I_{\gamma+}^{(1-\beta)(1-\alpha)} f \right) \right)(t) \tag{10}$$

for functions for which the expression on the right hand side exists.

The fractional Riemann – Liouville derivative is a special case of eq. (10) corresponding to $\beta = 0$, namely

$$D_{\gamma+}^{\alpha,0} f(x) = \frac{d}{dx} I_{\gamma+}^{1-\alpha} f(x) \tag{11}$$

where $0 < \alpha < 1$.

Another definition introduced by Liouville [14] in 1832, but often referred to as "the Caputo approach", corresponds to the fractional derivative of order α and type 1 as defined in eq. (10) and has proved to be very popular among engineers, especially as far as the field of viscoelasticity is concerned. It reads

$$D_{\gamma+}^{\alpha,1} f(x) = I_{\gamma+}^{1-\alpha} \frac{d}{dx} f(x) = \frac{1}{\Gamma(1-\alpha)} \int_{\gamma}^{x} \frac{f'(u)}{(x-u)^{\alpha}} du \tag{12}$$

where $0 < \alpha < 1$. This is a far more restrictive definition than the previous one, in that it demands that the derivative of $f(x)$ be absolutely integrable.

It is crucial to note that the different definitions of the fractional derivatives and integrals have a different physical meaning. It is therefore of great significance that care is taken, when entering the field of applications. One example of this fact is the connection of the fractional derivatives to continuous time random walks. Eq.(13) has a rigorous relationship with continuous time random walks, whereas the solution of eq.(14) does not admit a probabilistic interpretation [15].

$$D_{0+}^{\alpha,1} f\left(x,t\right) = C_{\alpha} \frac{\partial^2 f\left(x,t\right)}{\partial x^2} \tag{13}$$

$$D_{0+}^{\alpha,0} f\left(x,t\right) = C_{\alpha} \frac{\partial^2 f\left(x,t\right)}{\partial x^2} \tag{14}$$

where C_{α} is a fractional diffusion constant.

4 PREVIOUS WORK

Pachepsky et al. [5], following the scaling deviations observed in experiments from the scaling resulting from the Richards equation (cf. Table 1 of that reference) considered the equation

$$D_{0+}^{\alpha,0}\theta = \frac{\partial}{\partial x}\left(D_{\alpha}\left(\theta\right)\frac{\partial\theta}{\partial x}\right) \tag{15}$$

replacing the derivative with respect to time with a fractional one. Consequently they attempted a solution of the resulting time-fractional absorption equation by inserting the similarity variable from eq. (8) and transforming the equation into an ordinary differential equation, as was done by Philip, who introduced the similarity transform in the Richards equation. In an attempt to reproduce the results, we found that the transformation of eq. (15) into an ordinary fractional differential equation is not possible in the same way as in the case $\alpha = 1$. This is because the authors assumed the following relationship to hold:

$$D_{0+}^{\alpha,0}\theta = \frac{d\theta}{d\xi} D_{0+}^{\alpha,0}\xi \tag{16}$$

which leads to the ordinary fractional differential equation:

$$\frac{d}{d\xi}\left(D\left(\theta\right)\frac{d\theta}{d\xi}\right) - \frac{\Gamma\left(1-\alpha/2\right)}{\Gamma\left(1-3\alpha/2\right)}\xi\frac{d\theta}{d\xi} = 0 \tag{17}$$

Let as assume as a counterexample that $\theta = t^a$, $\xi = t^b$ .Then, for the eq. (16) the following relationship should hold for all values of b:

$$z\left(b\right) = \frac{1}{b}\frac{\Gamma\left(1+b\right)}{\Gamma\left(1+b-a\right)} = const \tag{18}$$

However, as can be seen in Fig. 2 this is not true. This finding gives rise to serious doubts concerning the validity of the numerical solution presented in [5]. An additional implication is the fact that the equation considered would in fact require an initial condition of integral type, which is not provided and in experimental situations is hard to obtain.

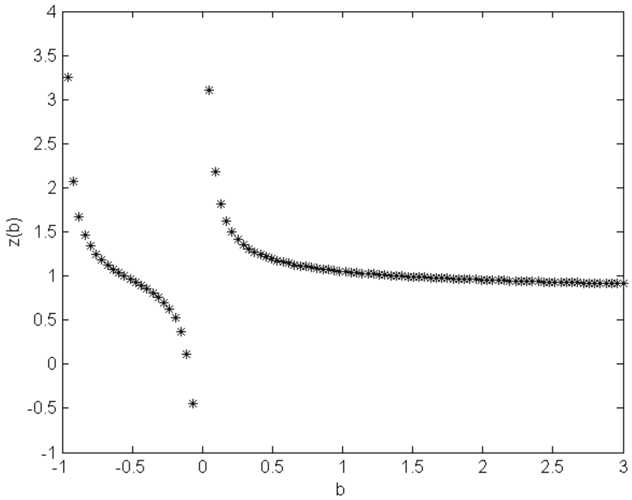

Figure 2: Counterexample demonstrating the inapplicability of the "chain rule", used in eq. (16)

5 FRACTIONAL RICHARDS EQUATION

The derivative of order equal to unity may be defined as follows

$$\frac{d}{ds} f(s) = \lim_{t \to 0} \frac{f(s) - f(s-t)}{t} = -\lim_{t \to 0} \frac{\mathrm{T}(t) f(s) - f(s)}{t} \tag{19}$$

which identifies $-d/dt$ as the infinitesimal generator of time translations defined as

$$\mathrm{T}(t) f(s) = f(s-t) \tag{20}$$

As shown by one of us [7], fractional derivatives arise respectively as the infinitesimal generators of coarse grained time evolutions

$$T_\alpha(t) f(s) = \int_0^\infty \mathrm{T}(u) f(s) h_\alpha\left(\frac{u}{t}\right) \frac{du}{t} \tag{21}$$

where t is considered as a duration of time and therefore it is always positive, and h_α is a one-sided stable law [7]. The order α of the derivative lies between zero and unity, and gives a quantitative measure for the decay of the averaging kernel h_α. The case $\alpha \neq 1$ indicates that memory effects and history dependence may become important.

Taking into consideration the nature of the problem and the initial conditions provided, it is obvious that we need to consider a fractional derivative of type $\beta = 1$, which would result in the following equation

$$D_{0+}^{\alpha,1} \theta(t,x) = \frac{\partial}{\partial x}\left(D_\alpha(\theta) \frac{\partial \theta(t,x)}{\partial x} \right) \tag{22}$$

with initial condition

$$\theta(0,x) = \tilde{\theta}(x) \tag{23}$$

where D_α is the fractional diffusivity and is in general dependent on θ. From this point on we will refer to eq. (22) as the fractional Richards equation.

6 NUMERICAL METHOD

For the solution of eq. (22) we will make use of an Adams-Bashforth-Moulton algorithm introduced by

Diethelm and Freed[16]. Eq. (22) is rewritten as a weakly singular Volterra equation of the second type

$$\theta(t,x)=\theta(0,x)+\frac{1}{\Gamma(\alpha)}\int_0^t (t-u)^{\alpha-1}\frac{\partial}{\partial x}\left(D_\alpha \frac{\partial\theta}{\partial x}\right)du \tag{24}$$

Considering an equidistant mesh

$$\theta_{n+1}(x)=\tilde{\theta}(x)+\frac{1}{\Gamma(\alpha)}\left(\sum_{j=0}^{n} a_{j,n+1} f\left(t_j,x,\theta_j(x)\right)+a_{n+1,n+1} f\left(t_{n+1},x,\theta^P_{n+1}(x)\right)\right) \tag{25}$$

where the predictor $\theta^P_{n+1}(x)$ is evaluated by the relationship

$$\theta^P_{n+1}(x)=\tilde{\theta}(x)+\frac{1}{\Gamma(\alpha)}\sum_{j=0}^{n} b_{j,n+1} f\left(t_j,x,\theta_j(x)\right) \tag{26}$$

and the constants are evaluated as follows

$$a_{j,n+1}=\begin{cases}\dfrac{h^\alpha}{\alpha(\alpha+1)}\left(n^{\alpha+1}-(n-\alpha)(n+1)^\alpha\right) & if\ \ j=0\\ \dfrac{h^\alpha}{\alpha(\alpha+1)}\left((n-j+2)^{\alpha+1}-2(n-j+1)^{\alpha+1}+(n-j)^{\alpha+1}\right) & if\ 1\le j\le n\\ \dfrac{h^\alpha}{\alpha(\alpha+1)} & if\ \ j=n+1\end{cases} \tag{27}$$

$$b_{j,n+1}=\frac{h^\alpha}{\alpha}\left((n+1-j)^\alpha-(n-j)^\alpha\right).$$

$f(t,x,\theta)$ signifies $\frac{\partial}{\partial x}\left(D_\alpha \frac{\partial\theta}{\partial x}\right)$, and for its evaluation finite elements will be used.

7 RESULTS

The fractional Richards equation, namely eq. (22), was solved by means of the numerical method presented in section 6. For the fractional diffusivity function we assumed

$$D_\alpha(\theta)=D_\alpha \tag{28}$$

where $D_\alpha = 0.1\,cm^2/min^\alpha$. The initial condition was assumed to be a step function given as

$$\tilde{\theta}(x)=\begin{cases}c_1, & x=0\\ c_2, & x>0\end{cases} \tag{29}$$

where $c_1 = 0.6$ and $c_2 = 0.2$.

In Figs. (3a) and (3b) the volumetric moisture content as a function of the distance from the beginning of the soil column is shown for the fractional Richards equation and Richards equation respectively. The curves displayed are isochrones corresponding to times equal to 0, 100, 200, 300, 400, 500, 600, 700, 800, 900 and 1000 min. The lowermost curve corresponds to the initial conditions, whereas the uppermost to time equal to 1000 min. For the case of the fractional Richards equation these results were achieved for order of the fractional derivative equal to 0.9. As can be seen in this case the process appears indeed to be slower than evaluated by the Richards equation and could therefore be termed as sub-diffusive.

In Fig 3(a) we plot x versus t , where x and t solve the equation

$$\theta(t,x)=0.3. \tag{30}$$

Here $\theta(t,x)$ is the solution of eq. (22) for $\alpha = 0.9$, $D_\alpha(\theta)$ given in eq. (28) and initial conditions as in eq. (29).

In Fig. 4(b) the isochrones of volumetric moisture content as a function of x are exhibited for different values of the fractional derivative and time equal to 1000 min. The curve closest to the axis corresponds to α =0.70, whereas the uppermost curve corresponds to the classical Richards equation.

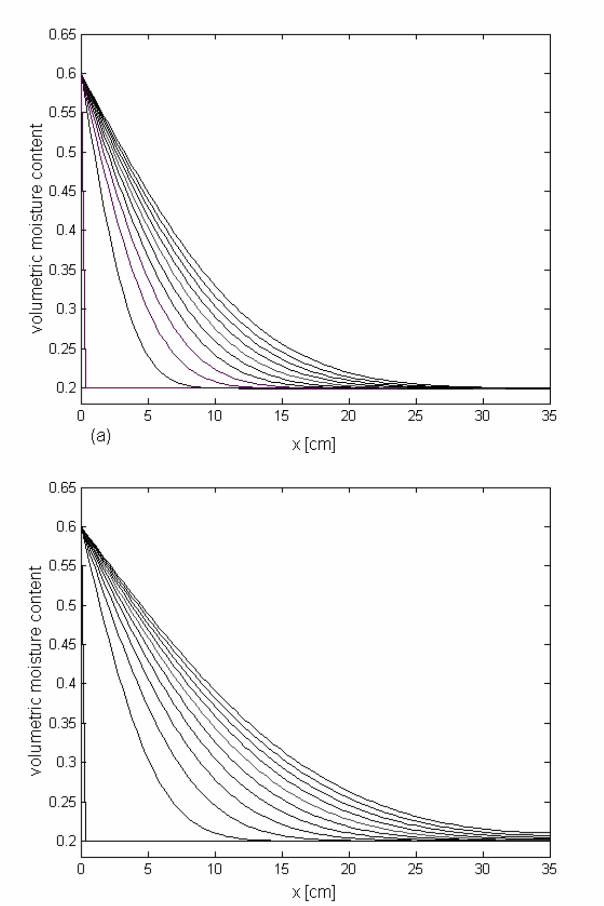

Figure 3: Isochrones of the volumetric moisture content $\theta(t,x)$ as a function of x for t =0, 100, …, 1000 min and initial conditions given by eq. (29). The uppermost curve corresponds to t =1000 min, whereas the one closest to the axis to the initial conditions. (a) Fractional Richards eq. (22) with $D_\alpha(\theta) = 0.1\,cm^2 / min^\alpha$; (b) Richards equation eq.(6) with $D(\theta) = 0.1\,cm^2 / min$.

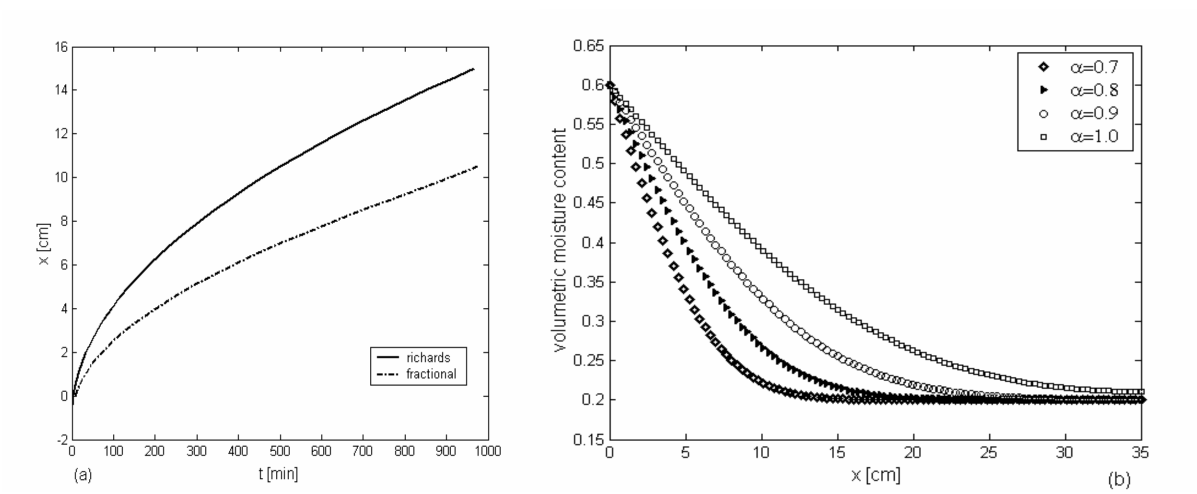

Figure 4: (a) Plot of the positions in time and space at which a volumetric moisture content $\theta(t,x)$ equal to 0.3 was observed for the Richards and the fractional diffusion equation, that is the solution of eq.(30); (b) The

volumetric moisture content $\theta(t,x)$ as a function of x is exhibited for different values of the fractional derivative α, with initial conditions given by eq. (29), $D_\alpha(\theta)$ given in eq. (28) and t equal to 1000 min.

8 CONCLUSIONS

The present study has shown that fractional calculus could be used to model the saturation front in partially saturated porous media in cases of subdiffusive behavior. It is important however that the right type of fractional derivative is introduced and the proper initial conditions are considered. Further on, it must be kept in mind that this approach has so far no proven connection neither to continuum mechanics nor to continuous time random walk theory and can be termed as phenomenological.

To further establish the possibility of using fractional derivatives to better model anomalous diffusion behavior of water in porous media, it is important that the relationship of the classical diffusivity to the fractional diffusivity is investigated and that work similar to the above for the case of varying diffusivity is produced, as we encountered numerical instability, when the exponential law, eq. (5), was implemented. It would also be of great interest to investigate the relationship between the movement of water in soil and the continuous time random walk with long-tailed power law distribution of waiting times.

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REFERENCES

[1] Jacques, D., Šimůnek, J., Timmerman, A., Feyen, J. (2002), "Calibration of Richards' and convection–dispersion equations to field-scale water flow and solute transport under rainfall conditions", Journal of Hydrology 259, No 1-4, pp. 15-31.

[2] Lewandowska, J., Auriault, J.-L. (2004), "Modelling of unsaturated water flow in soils with highly permeable inclusions", Comptes Rendus Mecanique 332, No 1, pp. 91-96.

[3] Van Dam, J.C., Feddes R. A. (2000), "Numerical simulation of infiltration, evaporation and shallow groundwater levels with the Richards equation", Journal of Hydrology 233, No 1-4, pp. 72-85.

[4] Gerolymatou E. (2004), *Simulation of the saturation front in partially saturated porous media,* Diploma Thesis, Faculty of Applied Mathematics and Physics, National Technical University of Athens.

[5] Pachepsky Y., Timlin D., Rawls W. (2003), "Generalized Richard's equation to simulate water transport in unsaturated soils", Journal of Hydrology 272, pp. 3-13.

[6] Ross, B. (Editor) (1975), *Fractional calculus and its applications, Lecture Notes in Mathematics #457,* Springer Verlag.

[7] Hilfer R. (2000), *Applications of fractional calculus in Physics*, World Scientific, Singapore.

[8] Zaslavsky G.M. (2002), "Chaos, fractional kinetics and anomalous transport", Physics Reports 371, pp. 461-580.

[9] Pachepsky Y., Timlin D., Rawls W. (2003), "Errata to generalized Richard's equation to simulate water transport in unsaturated soils", Journal of Hydrology 279, pp. 290.

[10] Philip J. R. (1969). "Theory of infiltration", Advances in Hydroscience 5, pp 215-296.

[11] Hilfer R. (1998), "Macroscopic Equations of Motion for Two Phase Flow in Porous Media", Physical Review E 58, pp 2090.

[12] Hilfer R. and Besserer H. (2000), "Macroscopic Two Phase Flow in Porous Media", Physica B 279, pp 125.

[13] Hillel D. (1980), *Applications of soil Physics*, Academic Press, New York.

[14] Liouville J. (1832), "Mémoire sur quelques questions de géométrie et de mécanique, et sur un nouveau genre de calcul pour résoudre ces questions", Journal de l'École Polytechnique 13, pp 1-66.

[15] Hilfer R. (2000), "Fractional diffusion based on Riemann-Liouville fractional derivatives", Jour. Phys. Chem. B 104, pp 3914-3917.

[16] Diethelm K. and Freed A. (1999), "On the solution of nonlinear fractional order differential equations used in the modeling of viscoplasticity", Scientific Computing in Chemical Engineering II—Computational fluid dynamics. In: F. Keil, W. Mackens, H. Voß and J. Werther, Editors, *Reaction Engineering, and Molecular properties*, Springer, Heidelberg, pp. 217–224.