Novel solution of the diffusion equation utilizing optimization through genetic algorithm

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Abstract: - The horizontal movement of water in a porous unsaturated medium is considered. An analytical expression is given for the diffusion coefficient that appears in the governing nonlinear partial differential equation. This expression contains adjustment parameters, allowing fitting to diffusion measurements. Four sets of such measurements of the pertinent literature were used for this fitting and for examining the validity of the model. The same procedure was employed to another expression of the literature for the diffusion coefficient and comparisons were made. The results showed that the diffusion expression presented in this paper exhibited a better fit (with respect to the relative mean square error) to the experimental data, compared to the expression of the literature. The calibration problem was treated by a combination of a genetic algorithm and the Nelder-Mead method. The expression of this paper for the analytical diffusion coefficient is based on a transformation of a corresponding expression for the moisture profile and, after the parameters' determination, moisture profiles and sorptivity become readily available.

Key-Words: - diffusion, unsaturated flow, fitting, genetic algorithm, soil moisture profile, Nelder-Mead method

1 Introduction

Water flow in an unsaturated medium or simply unsaturated flow is a particular case of water flow within a porous medium, the pores of which are partly filled with water and partly with air. Unsaturated flow is the mode of flow prevailing in the space above the phreatic horizon of groundwater bodies and it affects, among other things, water uptake by plant roots. Unsaturated flow is an essential component of such areas as Hydrology, Irrigation Engineering and Soil Mechanics. The study of unsaturated flow dates back at least to 1907 [1] with another notable early contribution by Gardner [2]. Richards [3] is credited with extending Darcy's law to unsaturated flow. However, a systematic study of water movement in unsaturated media is due to Childs [4]. A more modern review of the physical processes occurring in the unsaturated zone is given by Nimmo [5].

Quantitative analysis and simulation of unsaturated flow presents difficulties, as the respective differential equations, of the Fokker – Planck type, are nonlinear, with no exact solutions generally available. They are handled by means of numerical techniques and analytical or semi-analytical approximations ([6], [7], [8]).

The nonlinear partial differential diffusion equation applies in the case of horizontal unsaturated flow and its solution depends on knowledge of the diffusion coefficient D, various forms of which have been presented in the literature ([9], [10]).

Typically, the expressions for D contain a number of parameters that need to be determined. This is done in the framework of a calibration process, leading to an inverse problem approach, according to which the differential equation is solved by using trial values of the parameters. The profiles that result are compared to experimental measurement results and the trial values are then improved in the course of appropriate least-squares minimization procedures. Once the diffusion expression is fully determined, problems with similar geometrical and physical conditions can be handled by direct solution of the governing equation.

In this paper an alternative approach is presented. An empirical analytical four-parameter expression for the unsaturated flow moisture content profiles has been proposed in a previous work [11]. Based on this expression and the form of the governing diffusion equation, a corresponding expression for the diffusion coefficient is derived, that contains the same parameters as the profile expression. Subsequently, the expression for D is calibrated against experimental data for the diffusion coefficient. In order to carry out comparisons, the same data are used for the calibration of another established diffusion coefficient of the literature [9]. The comparisons are based on several data sets of the literature and, in all cases, the present expression gave better results.

After the determination of the four parameters of the function, moisture profiles and sorptivity are readily analytically available, without repeating the solution of the differential equation.

For the minimization problem that arose in the calibration process, a hybrid optimization scheme was employed in order to address the issue of a global optimization. The scheme consisted of a genetic algorithm in order to approximate the location of the minimum and of the Nelder-Mead method that was used to locally improve the estimate given by the genetic algorithm [12].

2 Problem Formulation

The one-dimensional horizontal movement of water in an unsaturated medium is governed by the diffusion nonlinear equation ([3],[13]):

$$\frac{\partial\theta}{\partial t}=\frac{\partial}{\partial x}\left[D(\theta)\frac{\partial\theta}{\partial x}\right],\quad 0<x<\infty \tag{1}$$

where θ is the soil moisture content as a function of time t and space x.

The diffusion coefficient D is assumed to be a function of θ [14].

The initial and boundary conditions are as follows:

$$t=0:\quad \theta(x,t)=\theta_i \quad x>0$$
$$x=0:\quad \theta(x,t)=\theta_0 \quad t>0$$
$$x\to\infty:\quad \theta(x,t)=\theta_i \quad t>0$$

By means of the Boltzmann transformation

$$\lambda = x\cdot t^{-1/2} \tag{2}$$

the above partial differential equation (1) is reduced to the following ordinary differential equation:

$$-\frac{1}{2}\frac{d\theta}{d\lambda}=\frac{d}{d\lambda}\left[D(\theta)\frac{d\theta}{d\lambda}\right] \tag{3}$$

with boundary conditions:

$$\lambda=0:\quad \theta(\lambda)=\theta_0$$
$$\lambda\to\infty:\quad \theta(\lambda)=\theta_i$$

Evangelides et al [3] presented an empirical approximate relation for the profile $\theta(\lambda)$ that underlies the above Equation (3):

$$\theta(\lambda)=A-B\tan^{-1}(C\lambda-D) \tag{4}$$

where A, B, C and D are parameters to be determined.

The expression (4) can be utilized to find a corresponding expression for $D(\theta)$. By integrating (3),

$$-\frac{1}{2}\int_{\theta_i}^{\theta}\lambda d\theta = D(\theta)\frac{d\theta}{d\lambda}.$$

Therefore,

$$D(\theta)=-\frac{1}{2}\frac{d\lambda}{d\theta}\int_{\theta_i}^{\theta}\lambda d\theta \tag{5}$$

By substituting expression (4) into (5) and rearranging,

$$D(\theta)=\frac{1}{2BC}\left(1+\tan^2\frac{A-\theta}{B}\right)\cdot \left[\frac{D}{C}(\theta-\theta_i)+\frac{B}{C}\ln\frac{\cos((A-\theta)/B)}{\cos((A-\theta_i)/B)}\right] \tag{6}$$

The above Equation (6) gives an analytical expression for $D(\theta)$. This expression is necessary for the solution of the partial (1) or of the ordinary differential equation (3).

Empirical expressions for $D(\theta)$ have appeared in the literature. A well-known such expression is due to Ahujia and Schwarzendruber [4]:

$$D(\theta)=a\theta^m(\theta_c-\theta)^n \tag{7}$$

where θ is moisture content and a, m and n are parameters to be determined.

Suppose that a set of experimental measurements of D versus θ $\{\theta_j, D_j\}$, j=1,2,..,N are given.

Then, the problem is to calibrate expression (6) and expression (7), so as to fit these data.

3 Problem Solution

Let $D(\theta; A, B, C, D)$ and $D(\theta; a, m, n)$ denote the expressions (6) and (7) respectively. Then the relative mean square errors used for evaluating the goodness of fittings will be given by Equations (8) and (9) below:

$$\text{rel.mse1}(A,B,C,D)=\frac{\sum_{j=1}^{N}[D(\theta_j;A,B,C,D)-D_j]^2}{\sum_{j=1}^{N}(D_j-D_{av})^2} \tag{8}$$

$$\text{rel.mse2}(a,m,n) = \frac{\sum_{j=1}^{N}[D(\theta_j;a,m,n) - D_j]^2}{\sum_{j=1}^{N}(D_j - D_{av})^2} \quad (9)$$

where $D_{av} = \sum_{j=1}^{N} D_j / N$

The quantities rel.mse1 and rel.mse2 can be considered as objective functions to be minimized in order to determine the respective parameters. Based on the values of rmse1 and rmse2 comparisons can be made as to the fitting provided by expression (6) of this paper versus the established expression (7) of the literature.

The optimization problem that results from the fitting requirements is solved in this paper by a hybrid process that includes a genetic algorithm and the Nelder-Mead method. The former locates the area of the minimum and the latter performs a local search. The genetic algorithm was run for 300 generations with a crossover probability of 0.7, mutation probability of 0.04 and population size equal to 50. The sample space for all parameters extended from 0.01 to 12.00.

4 Results and discussion

Muralli et al [10] presented experimental data for $D(\theta)$ for four soil samples, labeled as 207, 329, 331 and 338. They adjusted the parameters of expression (7) to these sets of data. In this paper both the parameters a, m and n of expression (7) and the parameters A, B, C and D of expression (6) are adjusted to the four sets of data and comparisons are made, as to compare the fitting achieved by the two expressions.

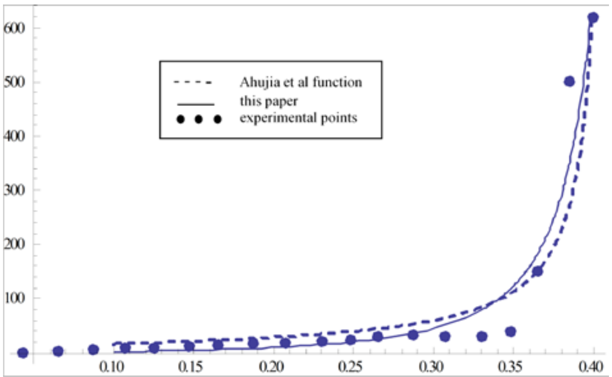

Figure 1. Data fitting for data set 207
rel.mse1=0.0226756 (this paper)
relmse2=0.0121794 (Ahuja et al)

Figures 1-4 show the curves corresponding to the two expressions, along with the values of the relative mean square errors. The results in all four soil samples show a better fitting of the expression of this paper, compared to the expression of Ahuja et al [4].

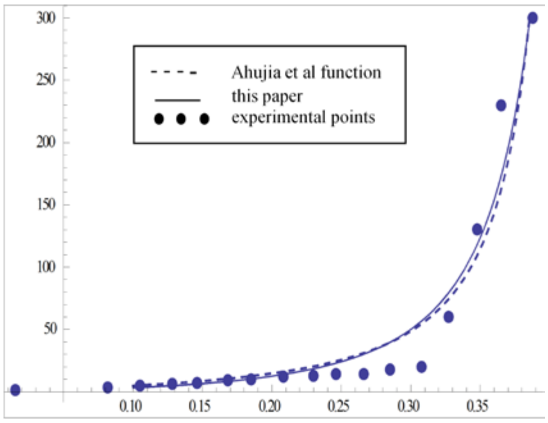

Figure 2. Data fitting for data set 329
relmse1=0.0019981 (this paper)
relmse2=0.0055862 (Ahuja et al)

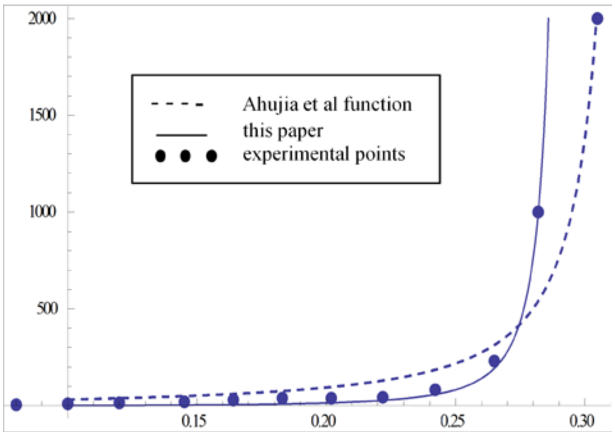

Figure 3. Data fitting for data set 331
relmse1=0.03624 (this paper)
relmse2=0.06228 (Ahuja et al)

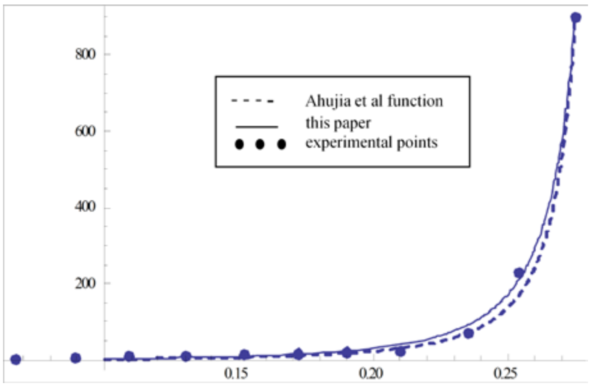

Figure 4. Data fitting for data set 338
relmse1=0.053199 (this paper)
relmse2=0.066897 (Ahuja et al)

The parameter values of the two expressions are given in Tables 1 and 2.

Table 1. Optimal parameter values for the expression (6) of this paper

Data set	A	B	C	D
207	2.061995	1.05279	1.43525	11.26057
329	2.64128	0.29880	0.85423	10.62598
331	0.80522	0.29671	0.24955	6.63309
338	3.37916	1.86246	2.32065	30.44958

Table 2. Optimal parameter values for the expression (7)

Data set	a	m	n	θ_c
207	9.41096	0.25134	0.97737	0.41
329	4.11093	1.58464	1.77387	0.29
331	7.57018	0.31629	1.42827	0.32
338	6.19290	0.83877	1.50426	0.43

The better fitting is not the only benefit offered by the expression of Equation (6). By obtaining the values of the parameters A, B, C, D, the profile given Equation (4) becomes readily available, as well as the sorptivity and the cumulative infiltration. The latter quantities are given by the formulas:

$$S=\int_{\theta_i}^{\theta_0}\lambda d\theta=\frac{D}{C}(\theta_0-\theta_i)+\frac{B}{C}\ln\left[\frac{\left|\cos\frac{\theta_0-A}{B}\right|}{\left|\cos\frac{\theta_i-A}{B}\right|}\right] \tag{10}$$

$$I=S\sqrt{t} \tag{11}$$

5 Conclusions

An analytical expression was given for the diffusion coefficient contained in the nonlinear diffusion equation that models the horizontal movement of water in an unsaturated medium. That expression was derived from an analytical expression representing soil moisture profile. The four parameters contained in the diffusion expression were adjusted to experimental measurements and the results proved to be superior to those attained by another diffusion expression of the literature. Moreover, the requisite moisture profiles can be readily obtained, as well as the sorptivity and cumulative infiltration, without the need to solve the differential equation again. This constitutes a novel approach toward the management of the horizontal unsaturated flow problem. The genetic algorithm employed for the optimization problem permitted finding suitable initial values for the adjustment parameters, in order to obtain improved final results via local search methods.

References:

[1] Buckingham, E. Studies on the movement of soil moisture. *U.S. Dept of Agriculture, Government Printing Office*, Washington, 1907.
[2] Gardner, W. The movement of soil moisture. *Soil Science*, vol 11, issue 3, pp 215-233, 1921
[3] Richards, L. Capillary conduction of liquids through porous mediums. *Physics 1*, 1931, pp 318-333.
[4] Childs, E.C. An introduction to the physical basis of soil water phenomena. *John Wiley and Sons*, New York, 493 p.
[5] Nimmo, J.R. Unsaturated Zone Flow Processes in *Anderson M.G. and Bear J. Eds. Encyclopedia of Hydrological Sciences: Part 13 – Groundwater*, Chichester, UK, Wiley, v. 4, pp.2299-2322, 2005.
[6] Tzimopoulos, C. Finite elements solution of porous media flow. *Finite Elements in Water Resources, Proceedings of the 2nd International Conference*, Imperial College, London, Pentech Press, 1978.
[7] Tolikas, P.K., Tzimpoulos, C. and Tolikas D.K. Horizontal absorption of water by soils with variable diffusivity. *Journal of Hydrology*, 58, pp. 123-129, 1982.
[8] Tolikas, P.K and Sidiropoulos E. Nonlinear diffusion with linearly varying diffusivity. Journal of Hydrology, 71, pp.181-190, 1984.

[9] Ahuja, L.R. and Swartzendruber, D.,. An improved soil water diffusivity function. *Soil. Sci. Soc. Am. Proc.*, vol. 36, 1972 pp.9-14
[10] Muralli, V., Krishna Murti, G.S.R and Sinha, A.K,. Note on the three parameter functions for soil water diffusivity water content relationship. *Aust. J. Soil Res.*, vol.17, 1979, pp. 361-366.
[11] Evangelides, C., Tzimopoulos, C. and Arampatzis, G.,. Flux-saturation relationship for unsaturated horizontal flow. *Soil Sci.*, vol. 170, 2005, pp. 671-679.
[12] Chelouah R. and Siarry, P. Genetic and Nelder-Mead algorithms hybridized for a more accurate global optimization of continuous multiminima functions. European Journal of Operational Research, 148, pp.335-348, 2003.
[13] Nielsen, D.R., Biggar, J.W. and Davidson, J.M.,., Experimental consideration of diffusion analysis in unsaturated flow problems, *Soil Sci. Soc. Am. Proc*, vol.26, 1962, pp. 107-111.
[14] Bruce, R.R. and Klute, A.,. The measurement of soil water diffusivity. *Soil Sci. Soc. Am. Proc.*, vol.20, 1956, pp.458-462.