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DETERMINATION OF SOIL HYDROLOGICAL PARAMETERS OF A MULTI-LAYERED LOESS COMPLEX USING HYDRUS-2D AND FIELD INFILTRATION EXPERIMENTS

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Abstract

The importance of the unsaturated zone as an integral part of the lithosphere for water flow and solute transport modelling has long been recognized. The hydraulic properties of the variably saturated zone are often comprehensively described by means of the van Genuchten–Mualem model. This paper deals with an inverse modelling approach using the software code HYDRUS-2D and field infiltration data for determination of the van Genuchten–Mualem parameters. For that purpose, laboratory and field hydraulic tests have been performed using respectively undisturbed core samples collected from a multi-layered loess complex and an in-situ borehole infiltration set-up in the same sediments near the town of Kozloduy, Northern Bulgaria. The obtained data was used to inversely estimate hydraulic properties with HYDRUS-2D at spatial scales much larger than the traditional laboratory-based analysis. The resulting large-scale parameters can be further implemented into water flow and solute transport models for more reliable assessment of radionuclide migration from nuclear facilities in the region of the town of Kozloduy, Northern Bulgaria.

Key words: variably-saturated zone, hydraulic properties, HYDRUS-2D

1. Introduction. The migration of contaminants in the lithosphere is a compilated and multi-process phenomenon [1–3]. It usually involves the combination of several physical and chemical processes such as convective mass transport,

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hydrodynamic dispersion, molecular diffusion, adsorption/desorption, ionic exchange, precipitation/dissolution, radioactive decay, etc. [4, 5]. Hence the relevant numerical simulators should incorporate all the above processes. Numerical modelling is further complicated when mass transport is through unsaturated media [6, 7]. The most popular approaches to the mathematical description of water flow and mass transport incorporate the Richards' equation for variably-saturated flow and the Fickian-based convection-dispersion equation for solute transport [5, 8, 9]. Therefore, the characterization of hydrological parameters and subsequent numerical modelling of water flow in the vadose zone is a key component in any contaminated site risk assessment. Accurate analysis of the unsaturated flow regime requires an investigation of the stratification in soil and sediment profiles and determination of layer specific hydraulic parameters by either laboratory on field tests [10–13]. This paper discusses the use of the HYDRUS-2D computer code [14] to determine vadose zone hydraulic parameters from borehole infiltration tests by inverse modelling. The 10-m deep soil profile investigated is located in Pleistocene loess complex near the town of Kozloduy, Northern Bulgaria.

2. Theory of variably saturated water flow. Water flow in variably saturated porous medium is often described by the Richards' equation [14]. For one-dimensional vertical flow this equation becomes

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

where θ is volumetric soil water content $[L^3 L^{-3}]$; t is time [T]; z is vertical coordinate (reference level for reading) [L]; K is hydraulic conductivity $[\mathrm{LT}^{-1}]$; h is soil water pressure head [L].

The solving of Eq. (1) requires knowledge of two highly nonlinear functions, the soil water retention curve $\theta(h)$ and the hydraulic conductivity function $K(h)$. One of the most popular and flexible closed-form equations describing the water retention curve was developed by van Genuchten [15] and is coupled mostly with the statistical pore size distribution model of Mualem [16], defined respectively as

$$\theta(h) = \begin{cases} \theta_r + \dfrac{\theta_s - \theta_r}{(1+(\alpha|h|)^n)^m} & h < 0 \\ \theta_s & h \geq 0 \end{cases} \tag{2}$$

$$K(h) = \begin{cases} K_s K_r(h) & h < 0 \\ K_s & h \geq 0 \end{cases} \tag{3}$$

$$K_r = S_e^l[1 - S_e^{1/m})^m]^2 \tag{4}$$

where θ and θ_s are respectively residual and saturated water content [L^3L^{-3}], α [L^{-1}], $n[-]$ and m ($m = 1 - 1/n$) are empirical constants defining the shape of the curves, h is soil water pressure head [LT^{-1}], l is empirical constant, assumed equal to 0.5, k is relative hydraulic conductivity [LT^{-1}], K_s is saturated hydraulic conductivity [LT^{-1}], and S_e is saturation degree given by $S_e = \dfrac{\theta - \theta_r}{\theta_s - \theta_r}[-]$.

According to the van Genuchten-Mualem model, knowledge of the five hydraulic characteristic parameters θ_r, θ_s, α, n and K_s hydraulic characteristic parameters allows quantification of the two functions and $K(h)$ [15]. The values of these parameters for a given soil can be determined by field and/or laboratory tests (see further). The software code HYDRUS-2D incorporates the above-mentioned relations in solving Richards' equation [14].

3. Methods for evaluation of soil hydraulic properties. ***3.1. Direct laboratory tests.*** The traditional method of determining the water retention function involves establishing a series of equilibriums between water in the soil sample and a body of water at known suction potential ψ_m equivalent to the soil water pressure head $h_m = -\psi_m/\rho_w g$) [17]. At each equilibrium, the volumetric volume content, θ, of the soil is determined and paired with a value of the pressure head, h_m, determined from the pressure in the body of water and the gas phase pressure in the soil. Each data pair (θ, h_m) is one point on a retention function. For a reliable description of the water retention curve, a sufficient number of points is required, usually more than six.

There are two variants of the laboratory approach for determination of the retention curve: 1) *a drainage curve* is mapped by establishing a series of equilibriums by drainage from saturated soil samples (zero pressure head); 2) *a wetting curve* is obtained by wetting dry samples (usually until saturation). In this study the first variant was applied.

The standard equipment for determining the retention function consists of two types: a sand box apparatus (Fig. 1*a*) and pressure cells (Fig. 1*b*). The sand box technique is used for pressure head values from saturation to pF 2 ($h_m = -100$ cm as pF $= -\log h_m$, cm), while the pressure cell method is used for drier conditions (> pF 2).

From the laboratory data of and θ and h_m, the parameters of the van Genuchten water retention function, θ_r, θ_s, α, n, may be obtained after inverse optimization with the RETC code [18]. Values for saturated hydraulic conductivity K_s are typically obtained by using the constant head method [19].

Several undisturbed 100 cm^3 soil samples were taken from the Quaternary-Pliocene loess complex in the Kozloduy NPP area. Hydraulic properties were measured following the above-mentioned laboratory procedures (for results see Fig. 2 and Table 1). Best-fit parameters θ_r, θ_s, α and n are shown on Table 2.

Due to spatial variability, the results of the laboratory tests made at small samples (the so-called cm-scale) may not accurately represent the vadose zone

Table 1

Measured soil hydraulic properties of undisturbed soil samples

Sample No	Soil description	Depth from the surface m	Total porosity $cm^3\,cm^{-3}$	Volumetric water content ($cm^3\,cm^{-3}$) at								
				pF 0	pF 0.5	pF 1	pF 1.5	pF 2	pF 2.3	pF 2.8	pF 3.4	pF 4.2
				–	–	–	–	–	–	–	–	–
U2	paleo-soil	7.5	0.477	0.402	0.394	0.384	0.365	0.330	0.275	0.209	0.191	0.141
U4	silty loess	10.0	0.473	0.470	0.441	0.435	0.423	0.393	0.333	0.222	0.136	0.100
U5	silty loess	11.5	0.480	0.451	0.441	0.435	0.423	0.398	0.346	0.285	0.136	0.104
U6	clayey loess	13.0	0.495	0.413	0.398	0.384	0.361	0.335	0.289	0.263	0.247	0.228
U7	clayey loess	14.0	0.488	0.413	0.404	0.391	0.371	0.344	0.315	0.268	0.262	0.256
U8	red clay	15.0	0.402	0.369	0.357	0.350	0.331	0.314	0.299	0.281	0.270	0.258
U9	red clay & gravel	16.3	0.417	0.411	0.403	0.402	0.400	0.393	0.359	0.313	0.294	0.266

water flow processes at the spatial profile scale [20]. For that reason, a series of hydraulic field tests were performed to better capture spatial variability and determine hydraulic properties at a degree commensurate with the scale of numerical modelling. Besides, several of the loess layers contained carbonate or gravel concretions that did not allow collection of undisturbed core samples.

3.2 Field infiltration tests for determination of the hydraulic parameters. Constant-head infiltration tests were carried out for determining field-

Table 2

Fitted van Genuchten moisture retention parameters (θ_s, α, n); parameter θ_r is fixed at zero; K_s is measured

Sample No (soil description)	θ_s	α	n	K_s
	$cm^3\,cm^{-3}$	m^{-1}	–	$m\,s^{-1}$
U2 (paleosoil)	0.402	3.3	1.177	1.75E-07
U4 (silty loess)	0.331	0.3	1.368	3.88E-07
U5 (silty loess)	0.442	0.6	1.356	4.63E-07
U6 (clayey loess)	0.418	22.9	1.082	1.25E-06
U7 (clayey loess)	0.420	22.8	1.071	5.02E-07
U8 (red clay)	0.377	69.1	1.044	5.29E-08
U9 (red clay & gravel)	0.410	2.1	1.081	2.12E-08

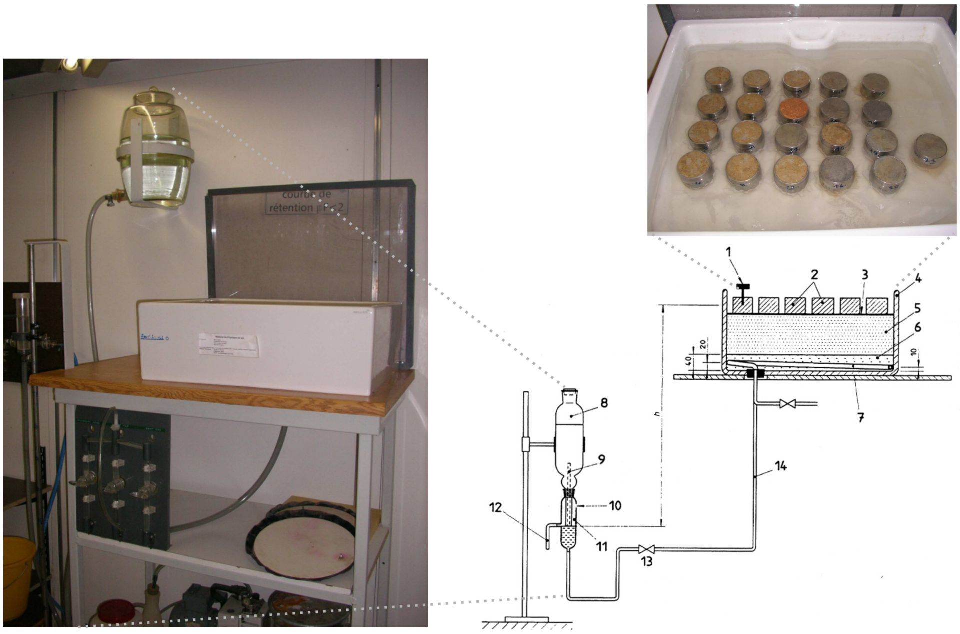

Fig. 1*a*. Sand suction table for soil water suction determination up to pF 2 [21]: 1 – tensiometer; 2 – soil core sample; 3 – nylon voile; 4 – ceramic sink; 5 – fine sand; 6 – coarse sand; 7 – drain system; 8 – reservoir; 9 – thin nylon tube; 10 – air inlet; 11 – levelling bottle; 12 – overflow; 13 – tap; 14 – flexible nylon tubing

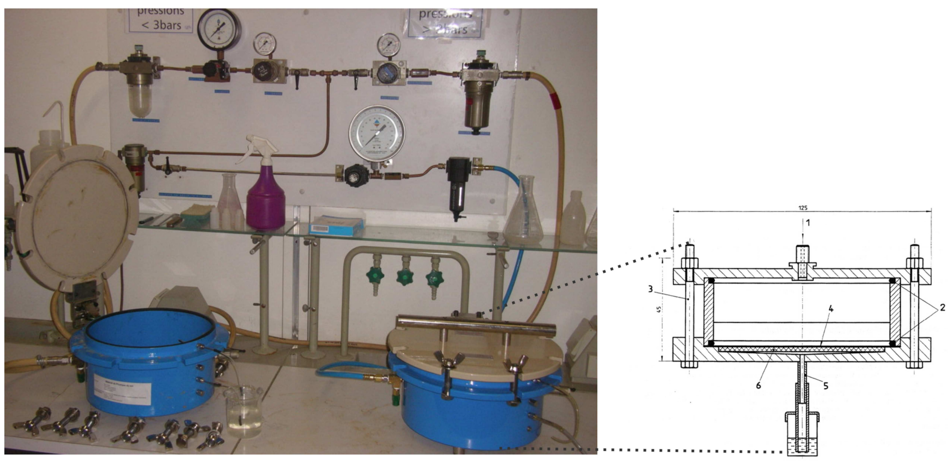

Fig. 1*b*. Pressure membrane cell for soil water suction determination > pF 2 [20]: 1 – air from compressor; 2 – O-rings; 3 – bolts; 4 – visking membrane; 5 – outflow pipe; 6 – sintered bronze plate

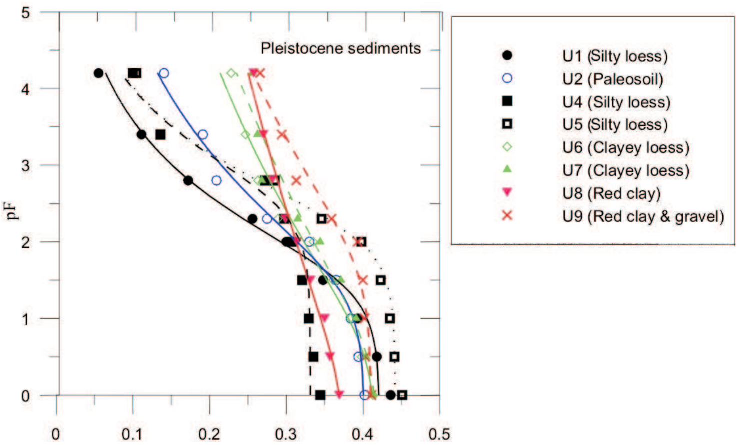

Fig. 2. Measured (symbols) and fitted van Genuchten moisture retention curves

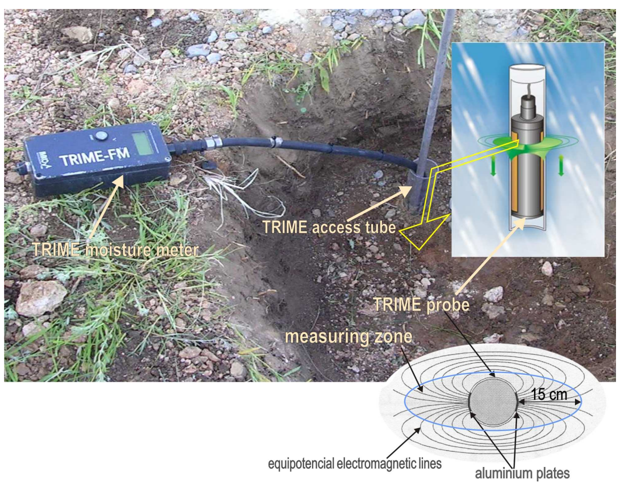

Fig. 3. Time-domain reflectometry apparatus (TRIME T3-44) for volumetric soil moisture measurements

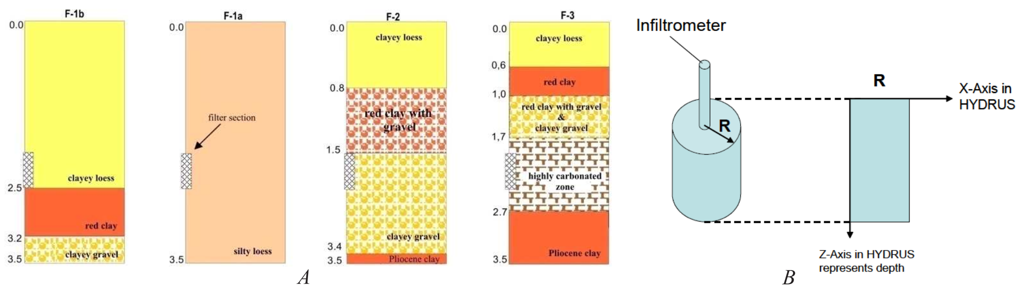

Fig. 4. *A*) Conceptual models used in the axisymmetric flow calculations. Vertical dimensions (in metres) refer to model coordinates. *B*) Axisymmetrical flow model with radially finite, 3D geometry, applied to each of the conceptual models

scale soil hydraulic properties. Four such tests were carried out up to 10 m depth in a Pleistocene loess complex located near the town of Kozloduy, Northern Bulgaria. Infiltration tests provided data on cumulative infiltration and progression of the wetting front in the initially unsaturated sediments surrounding the infiltrometers. A cylindrical time-domain reflectometry TRIME-IPH/T3 probe operated by the TRIME-HD device was used to measure water content variations with time during the progression of the wetting front. Special polycarbonate access tubes for the TRIME probe were installed at 0.3 to 0.5 m from the infiltrometers (Fig. 3).

By means of an inverse optimization routine implemented in the finite element code HYDRUS-2D, field-scale soil hydraulic parameters θ_r, θ_s, α and n were derived for particular layers. The inverse optimization is based on simulating the expected soil water redistribution history while adjusting the soil hydraulic parameters until the best possible agreement is obtained between measured and calculated cumulative infiltration and soil moisture profile. An axisymmetric model was developed in HYDRUS-2D for each of the four infiltrometers (Fig. 4*B*). The vertical dimension of the model was limited to the soil layers that would be immediately influenced by the infiltrating water (Fig. 4*A*). The simulation starts with "guess" or "trial" values of the soil hydraulic properties; these values may be estimated using pedotransfer functions based on particle size data, or by using some other prior information, such as the laboratory tests data.

Initial optimization with three parameters, α, K_s and n, showed high correlation between α and K_s, and a high standard error coefficient for n indicative of non-uniqueness of the solution. Therefore, the parameter n was excluded from being optimized. The automatic parameter optimization routine provided in HYDRUS-2D was invoked to further optimize the parameters α and K_s [14]. The parameter n is kept constant at its initial value of 2 (obtained from initial trial runs). The results from parameter optimization for each of the modelled infiltrometers F-1b, F-1a, F-2, and F-3 are shown on Table 3. Overall good fits were obtained with hydraulic parameters representative for several m3 of soil.

4. Conclusion. A series of laboratory and field investigations have been performed in order to characterize the unsaturated zone in Pleistocene loess sediments near the town of Kozloduy, Northern Bulgaria. The values of the van Genuchten model parameters have been estimated by laboratory and field tests. The laboratory data were analysed with the RETC code and produced best fit θ_r, θ_s, α and n parameters at the cm-scale. The same parameters have been successfully derived from a series of field borehole infiltration tests after inverse optimization with the computer code HYDRUS-2D. The field-based parameters are representative of a soil volume of several m^3 of soil.

Due to the small measurement scale of the laboratory test, at most a few hundred cubic centimetres, hydraulic properties determined on core samples may not entirely capture the large scale flow processes in heterogeneous and layered

Table 3

Parameter values from inverse optimization using HYDRUS-2D

Soil description	Parameter	Best fitted value	S.E. coefficient	Lower 95%	Upper 95%
Clayey loess* [F1b]	$\alpha[\mathrm{m}^{-1}]$	0.351	0.0354	0.2807	0.490
	$K_s[\mathrm{m\ s}^{-1}]$	6.03E-07	0.00144	0.0492	0.0549
	SSQ	0.0119			
	R^2	0.99685			
Red clay [F1b]	$\alpha[\mathrm{m}^{-1}]$	0.497	0.450	−0.395	1.389
	n	4.29			
	$K_s[\mathrm{m\ s}^{-1}]$	6.89E-07	0.0229	0.0140	0.105
	SSQ	0.0118			
	R^2	0.9969			
Silty loess* [F1a]	$\alpha[\mathrm{m}^{-1}]$	0.0586	0.00849	0.04177	0.0754
	$K_s[\mathrm{m\ s}^{-1}]$	5.20E-07	0.00068	0.0436	0.0463
	SSQ	0.00281			
	R^2	0.99939			
Clayey gravel* [F2]	$\alpha[\mathrm{m}^{-1}]$	3.00	1.167	0.7014	5.298
	$K_s[\mathrm{m\ s}^{-1}]$	1.06E-06	0.000739	0.089	0.0927
	θ_s	0.413	0.00011	0.411	0.416
	SSQ	0.00251			
	R^2	0.99935			
Highly carbonated zone* [F3]	$\alpha[\mathrm{m}^{-1}]$	2.683	2.288	−1.846	7.211
	$K_s[\mathrm{m\ s}^{-1}]$	1.88E-07	0.000246	0.01579	0.01677
	θ_s	0.354	0.0229	0.308	0.399
	SSQ	0.003907			
	R^2	0.9981			

*Parameter n is fixed at 2

sediments. Therefore, the use of a field-scale approach is the preferred option for obtaining hydraulic flow parameters representative of larger soil volumes typically used as grid elements in numerical models.

The field constant head infiltration test applied in the present study has proven to perform successfully especially for clayey gravel and highly-carbonated layers. Field-scale hydraulic parameters obtained at different locations were consistent, with little special variability. The use of a field infiltrometer set-up in which a relatively large volume of soil is affected by the constant head infiltration process average out the effects of special variability. The spatial scale of the measurements is further commensurate with the spatial dimensions of the discretization used in the finite element modelling of contaminant transport. The use of field infiltration data in the inverse optimization routine of the computer code HYDRUS-2D is a practical and reliable methodology to obtain field-scale hydraulic characteristics. The hydraulic parameters determined here can be readily used for a large scale calculation of flow patterns in variably-saturated media in the modelling of radionuclide migration in the region of Kozloduy NPP.

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