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# HYDRUS Software Applications to Subsurface Flow and Contaminant Transport Problems

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### Preface

These proceedings document presentations given at the Fourth International Conference on "HYDRUS Software Applications to Subsurface Flow and Contaminant Transport Problems," held in Prague, Czech Republic, March 21-22, 2013. Previous conferences in this series were held in Utrecht in 2005, in Prague in 2008, and in Tokyo, also in 2008. The conferences focus on the development and application of advanced numerical models simulating variably-saturated flow, heat transport, and the transport of various contaminants or other solutes (such as nutrients, pesticides, heavy metals, radionuclides, and pathogenic microorganisms) in soils and groundwater. The conferences are designed to bring together users of the HYDRUS family of codes, as well as of related software, to review and exchange information on various aspects of the codes, future enhancements of the software, and their application to a range of soil, environmental, hydrological, ecological and agricultural problems.

Since the first workshop in 2005, the community of HYDRUS users has been continuously growing as evidenced by the number of downloads (over 10,000 times each of the past several years) and visits to the HYDRUS web pages (on average several hundred each day). Hundreds of journal articles have now been published in which the HYDRUS codes have been used. Feedback from users such as those attending the HYDRUS conference has been extremely important in identifying particular strengths and weaknesses of the codes, and for defining additional processes or features that should be included in the models. Feedback is also continuously obtained from several discussion forums on the HYDRUS website, where users can submit questions or suggestions about the models.

These proceedings contain 41 contributions from mostly HYDRUS software users, covering a range of topics from the very fundamental to important practical applications. These proceedings, as well as those of previous HYDRUS conferences, can be downloaded freely from the HYDRUS website at <u>http://www.pc-progress.com</u>.

We would like to thank the Czech University of Life Sciences and PC-Progress for hosting the conference in Prague. Our appreciation goes also to the many participants who travelled to Prague from all continents. Special thanks are due to those that contributed to these proceedings. Published studies in which the codes have been used always provide useful information for new users. We believe that the software tools have served, and will continue to serve, an important role in especially vadose zone research.

The Editors

Jirka Šimůnek Rien van Genuchten Radka Kodešová

### Application of the HYDRUS (2D/3D) Inverse Solution Module for Estimating the Soil Hydraulic Parameters of a Quaternary Complex in Northern Bulgaria

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#### Abstract

Characterizing hydraulic properties of the unsaturated zone at spatial scales commensurate with the numerical model grid size is key to reliable predictive modeling of the fate and transport of contaminants in the environment. We used the HYDRUS (2D/3D) model and inverse modeling to determine the hydraulic properties of a 10-m deep vadose zone from borehole infiltration tests. The investigated soil profile is located in the Pleistocene loess complex near the town of Kozloduy, Northern Bulgaria, in the vicinity of the Kozloduy Nuclear Power Plant (NPP). Four constant-head infiltrometer tests were carried out several meters below the ground surface to determine the unsaturated hydraulic properties of a silty loess, clayey loess, clayey gravel, and a highly carbonated layer. Infiltration tests provided data on cumulative infiltration and the movement of the wetting front in the initially unsaturated sediments surrounding the infiltrometer. A cylindrical TRIME-IPH/T3 time-domain reflectometry probe was used to measure water content variations with time during the movement of the wetting front. An axisymmetric model was developed in HYDRUS (2D/3D) for each of the four infiltrometer tests. The inverse optimization routine implemented in HYDRUS (2D/3D) was used to determine field-scale soil hydraulic parameters  $\theta_r$ ,  $\theta_s$ ,  $\alpha$ , n, and  $K_s$  for all layers of interest. Results suggest the size of the affected volume of soil was large enough to reduce the effect of spatial variability and to produce effective field-scale hydraulic parameters that are relevant for prediction of large-scale, variably-saturated water flow and radionuclide migration pathways at the Kozloduy NPP site.

#### 1. Introduction

At present, only one nuclear power plant (NPP) is in operation in Bulgaria. Two reactors out of six are still in operation near the town of Kozloduy, while the remaining four were shut down in December 2002 (units 1 and 2) and December 2006 (units 3 and 4). A National Repository for Low and Intermediate Level Radioactive Waste (LILW) from all the units is foreseen to be built in the vicinity of the Kozloduy NPP. The investigated area represents an undulating landscape developed on Pliocene clay covered with loess sediments, with the groundwater table usually located in a clay formation at a depth of about 30 m (Antonov, 2002). For the purposes of a safety assessment for the LILW repository, an evaluation of radionuclide migration through variably-saturated, geological strata should be performed.

The fate and transport of contaminants in the geosphere is a multi-process phenomenon. It usually involves the combination of several physical and chemical processes, such as convective

mass transport, hydrodynamic dispersion, molecular diffusion, adsorption/desorption, ionic exchange, precipitation/dissolution, radioactive decay, etc. (Jacques et al., 2008; Mallants et al., 2011). Hence, the relevant numerical simulators should incorporate all the above processes. 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 convectiondispersion equation for solute transport (Mallants et al., 2011). Therefore, the characterization of hydrological parameters and subsequent numerical modeling 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 or field tests. When the soil is characterized by a complicated structure and texture, the results of laboratory tests carried out on small samples may not fully capture properties of the unsaturated zone (Mallants et al., 1997). Examples of successful determination of the soil hydraulic parameters via different types of field experiments, including for the purposes of migration analyses, can be found in Kodešová et al. (1999) and Gvirtzman et al. (2008). This paper discusses the use of the HYDRUS (2D/3D) (Šimůnek et al., 2006) computer code to determine by inverse modeling hydraulic parameters of the vadose zone from borehole infiltration tests. The investigated 10-m deep soil profile is located in the Pleistocene loess complex near the town of Kozloduy, Northern Bulgaria.

#### 2. Theory and Methods

Water flow in variably-saturated soils is described using the Richards equation. A onedimensional form is given as follows:

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

where  $\theta$  is the volumetric soil water content  $[L^3L^{-3}]$ , *t* is time [T], *z* is the vertical coordinate (from a reference level) [L], *K* is the unsaturated hydraulic conductivity  $[LT^{-1}]$ , and *h* is the soil water pressure head [L]. Numerical solution of Eq. (1) requires the knowledge of two highly nonlinear functions, namely the soil water retention curve,  $\theta(h)$ , and the unsaturated hydraulic conductivity function, *K*(*h*). One of the most popular and flexible equations describing  $\theta(h)$  was developed by van Genuchten (1980). When coupled with the statistical pore size distribution model of Mualem (1976), it gives a closed-form equation for *K*(*h*):

$$\theta(h) = \begin{cases} \theta_r + \frac{\theta_s - \theta_r}{\left(1 + \left(\alpha \left|h\right|\right)^n\right)^m} & h < 0 \\ \theta_s & h \ge 0 \end{cases}$$
(2)

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

where

$$K_{r} = S_{e}^{l} \left[ 1 - \left( 1 - S_{e}^{\frac{1}{m}} \right)^{m} \right]^{2}$$
(4)

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

$$S_e = \frac{\theta - \theta_r}{\theta_s - \theta_r} \tag{5}$$

According to the van Genuchten-Mualem model, knowledge of the five parameters  $\theta_r$ ,  $\theta_s$ ,  $\alpha$ , n, and  $K_s$  allows quantification of the two functions  $\theta(h)$  and K(h) (van Genuchten, 1980). The values of these parameters for a given soil can be determined using field and/or laboratory tests (Mallants et al., 2007; Antonov et al., 2012). The software code HYDRUS (2D/3D) incorporates the above-mentioned relations (Šimůnek et al., 2006). The automatic parameter optimization routine implemented in HYDRUS (2D/3D) was used to optimize the parameters  $\alpha$  and  $K_s$  (see *further*). The HYDRUS code adopts the minimization of the sum of squared residual (SSQ):

$$SSQ = \sum_{i=1}^{N} (q_{p,i} - q_{o,i})^2$$
(6)

where N is the number of the calibration points (note that here only the cumulative fluxes are used),  $q_{p,i}$  is the *i*th predicted value, and  $q_{o,i}$  is the *i*th observed value. The HYDRUS code uses the Marquardt-Levenberg optimization algorithm to minimize the objective function (6).

#### 3. Field Infiltration Tests – Results and Discussion

Constant-head infiltration tests were carried out for determining the field-scale soil hydraulic properties. Four such tests were carried out down to a depth of 10 m in the unsaturated Pleistocene loess complex. 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. A more detailed description of the field and technical equipment layout could be found in Mallants et al. (2007). By means of an inverse optimization routine implemented in the finite element code HYDRUS (2D/3D), field-scale soil hydraulic parameters  $\theta_r$ ,  $\theta_s$ ,  $\alpha$ , and n were derived for particular layers, namely silty loess, clayey loess, clayey gravel, and a highly carbonated zone. For cemented layers, such as the clayey gravel and the carbonated zone, collection of classical soil cores is not possible, leaving only field determination as a reliable option for determining hydraulic properties (Fig. 1). 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 profiles. An axisymmetric model was developed in HYDRUS (2D/3D) for each of the four infiltrometers (Fig. 2).



Figure 1. Carbonate concretions in the carbonated zone (left) and gravel concretions from the gravel layer (right).

The vertical dimension of the model was limited to the soil layers that would be immediately influenced by infiltrating water (Fig. 2). 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, e.g., laboratory tests data.



Figure 2. A) Conceptual models used in flow calculations. Vertical dimensions (in m) refer to model coordinates. B) An axisymmetrical quasi-3D model. C) Observed and calculated cumulative infiltrations.

An initial optimization with three parameters,  $\alpha$ ,  $K_s$ , and n, showed a high correlation between  $\alpha$  and  $K_s$ , and a high standard error coefficient for n, indicating non-uniqueness of the solution. Therefore, the n parameter was excluded from optimization. The parameter optimization routine provided in HYDRUS (2D/3D) was invoked to further optimize the parameters  $\alpha$  and  $K_s$ . The n parameter was kept constant at its initial value of 2 (obtained from initial trial runs). The results from parameter optimization for each of the modeled infiltrometers F-1b, F-1a, F-2, and F-3 are shown on Table 1. Overall good fits were obtained with hydraulic parameters being representative of several cubic meters of soil.

Soil	Parameter	Best fitted	S.E. coefficient	Lower 95%	Upper 95%
description		value			
	$\alpha$ [m <sup>-1</sup> ]	0.351	0.0354	0.281	0.490
Clavov loose*	$K_s [\mathrm{ms}^{-1}]$	6.03E-07	0.00144	0.0492	0.0549
Clayey locss	SSQ	0.0119	-	-	-
	$R^2$	0.997	-	-	-
	$\alpha$ [m <sup>-1</sup> ]	0.497	0.450	-0.395	1.39
	n [-]	4.29	-	-	-
Red clay	$K_s [\mathrm{ms}^{-1}]$	6.89E-07	0.0229	0.0140	0.105
	SSQ	0.0118	-	-	
	$R^2$	0.997	-	-	-
	$\alpha$ [m <sup>-1</sup> ]	0.0586	0.00849	0.0418	0.0754
Silty looss*	$K_s [\mathrm{ms}^{-1}]$	5.20E-07	0.00068	0.0436	0.0463
Sitty 10ess	SSQ	0.00281	-	-	-
	$R^2$	0.999	-	-	-
	$\alpha$ [m <sup>-1</sup> ]	3.00	1.17	0.701	5.30
	$K_s [\mathrm{ms}^{-1}]$	1.06E-06	0.000739	0.089	0.0927
Clavov graval*	$\theta_s [\mathrm{cm}^3 \mathrm{cm}^{-3}]^{**}$	0.431	0.00011	0.411	0.416
Clayey graver	SSQ	0.00251 (0.000605) <sup>**</sup>	-	-	-
	$\mathbb{R}^2$	0.999 (0.999)**	-	-	-
	$\alpha$ [m <sup>-1</sup> ]	2.68	2.29	-1.85	7.21
III ablas souls an ato d	$K_s [\mathrm{ms}^{-1}]$	1.88E-07	0.000246	0.0158	0.0168
rightly carbonated	$\theta_s [\mathrm{cm}^3 \mathrm{cm}^{-3}]$	0.354	0.0229	0.308	0.399
ZOIIC	SSQ	0.00391	-	-	-
	$R^2$	0.998	-	-	-

Table 1. Parameter values obtained by an inverse optimization using HYDRUS (2D/3D).

\*Parameter *n* is fixed at 2; \*\* when  $\theta_s$  fitted separately.

#### 4. Conclusions

Field investigations have been performed in order to characterize the unsaturated zone in the Pleistocene loess sediments near the town of Kozloduy, Northern Bulgaria. The values of the van Genuchten model parameters have been derived from a series of field borehole infiltration tests using an inverse optimization with the computer code HYDRUS (2D/3D). Due to the small measurement scale of the laboratory test and the inability to obtain core samples from strongly cemented layers, 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. Field-scale hydraulic parameters obtained at different locations were

consistent, showing only 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, averages out the effects of special variability. The use of field infiltration data in an inverse optimization routine of the computer code HYDRUS (2D/3D) is a practical and reliable methodology to obtain field-scale hydraulic characteristics. Additional modeling work is required in the implementation of the TRIME probe data into the objective function of the minimization procedure.

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