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**INNOVATIVE IN-SITU DETERMINATION OF UNSATURATED HYDRAULIC PROPERTIES IN
DEEP LOESS SEDIMENTS IN NORTH-WEST BULGARIA**

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ABSTRACT

In the framework of selecting a suitable site for final disposal of low- and intermediate level short-lived radioactive waste (LILW-SL) in Bulgaria, site characterization is ongoing at the Marichin Valog site, North-West Bulgaria. The site is characterized by a complex sequence of loess, clayey gravel, and clay layers, of which the first 30-40 m are unsaturated. Proper knowledge about unsaturated water flow and concomittant radionuclide transport is key input to safety assessment calculations. Constant-head infiltrometer tests were carried out at several meters below ground surface to determine the unsaturated hydraulic properties of silty loess, clayey loess, and clayey gravel layers. Individual infiltrometers were equipped with 0.5-m-long filter sections; the shallowest filter was from 2 to 2.5 m depth, whereas the deepest was from 9.5 to 10 m depth. Infiltration tests provided data on cumulative infiltration and progression of the wetting front in the initially unsaturated sediments surrounding the infiltrometer. A cylindrical time-domain reflectometry TRIME probe was used to measure water content variations with time during progression of the wetting front. Access tubes for the TRIME probe were installed at 0.3 to 0.5 m from the infiltrometer tubes. By means of an inverse optimization routine implemented in the finite element code HYDRUS-2D, field-scale soil hydraulic parameters were derived for all layers. Results show a great consistency in the optimized parameter

values, although the test sites were several meters apart. Apparently the size of the affected volume of soil was large enough to reduce the effect of spatial variability and to produce average field-scale hydraulic parameters that are relevant for large-scale predictions of flow patterns and radionuclide migration pathways.

INTRODUCTION

At present, the only nuclear power plant in operation in Bulgaria is located in Kozloduy. At Kozloduy, six reactor units exist, with four in operation, while two were shut down in December 2002 (WWER 440/230 units 1 and 2) as a result of an agreement between the Bulgarian Government and the European Union. Two further units are planned to be shut down in the beginning of 2007 (units 3 and 4). Units 3 and 4 are also 440 MW WWER reactors, while units 5 and 6 are 1000 MW WWER reactors. For the Kozloduy plant, the total volume of LILW-SL for surface disposal is estimated at ~60 000 m³.

The Bulgarian State Enterprise Radioactive Waste Management (SERAW) is currently investigating the suitability of three sites for disposal of LILW-SL. Two sites are located in the vicinity of the Kozloduy NPP, notably Brestova Padina and Marichin Valog. The third site is located in Belene, along the Danube river. Marichin valog is located at about 2.5 km to the west-southwest direction from the Kozloduy NPP, while the other sites are located at a greater distance.

At present the Marichin Valog site is the most extensively characterized site; this work is mainly done by the Geological Institute of the Bulgarian Academy of Sciences. Because of the existence of relatively thick unsaturated loess/clay formations at the potential repository site, detailed characterization of these layers is needed in view of a defensible site evaluation. This paper documents the initial steps of the characterization of the hydraulic properties of the unsaturated loess/clay formations. The results reported are the outcome of collective efforts of the Geological Institute of the Bulgarian Academy of Sciences and the Belgian Nuclear Research Centre (SCK•CEN), in the framework of a bi-lateral cooperation between both countries.

SITE DESCRIPTION

Topography and stratigraphy

The Marichin valog site is located in an undulating landscape (Fig. 1) developed on Pliocene clay covered with Quaternary sediments. The latter consists of two layers: silty loess and clayey loess with a variable thickness between 5 and 14 m, and a clayey gravel layer of about 2 m thickness whose base is the interface with the Pliocene clay (Fig. 1). The repository is planned to be founded on the top of the Pliocene clay layer (at an elevation of ~85 m above mean sea level), after the removal of the Quaternary sediments. The inclination of the interface between Pliocene clay and clayey gravel is in north-west – south-east direction. The presumed outlet of the catchment is the Ogosta river, which is at a distance of 8-9 km. A thin low-yield aquifer is formed in a 1.5-2 m thick sandy-silty intercalation within the Pliocene clay layer. A seepage zone exists at a distance of about 300-350 m northeast of the site, where the aquifer is intersected by the nearby valley (Fig. 1). The top of the site (borehole BH 34) is at approximately 100 m above mean sea level, whereas the lowest point in the valley is at 64 m, and the groundwater table is at 63 m above mean sea level.

At Marichin Valog two sites were equipped with infiltrometer devices for the determination of unsaturated hydraulic properties ([1], [2]). The sites are at an elevation of 96 m (no. 1) and 88 m (no. 2) above mean sea level. The second site was subdivided into two subsites, i.e. site 2 and 3, with one infiltrometer device being installed in each site. The two sites were chosen in such a way that the first site would have a maximum thickness of all stratigraphic layers, whereas in the second site the top layers would have a significantly reduced thickness, or were even absent, due to erosion. As a result, the depth to the presumed foundation layer for repository construction (Pliocene clay) would be about 3 m for the second site versus ~16 m for the first site. Since the primary objective of this study was to hydraulically characterize the last few meters of the layer above the foundation layer, a much shorter infiltrometer device was necessary in the second site compared to the first. The primary layer to be hydraulically characterized by in-situ tests was classified as clayey gravel, which was chosen because 1) the contrast in hydraulic conductivity with the underlying Pliocene clay (i.e. $\sim 10^{-7} - 10^{-6}$ m/s versus $10^{-10} - 10^{-9}$ m/s) presumably is large enough to generate an important lateral flow component (note the inclined interface between Pliocene clay and clayey gravel) which could dominate the long-term flow pattern in the loess hill with much horizontal longer flow paths compared to flow paths associated with vertical drainage, (2) the presence of gravel makes core sampling and subsequent laboratory determination on core samples problematic.

The objective of the in-situ test at the first site was to hydraulically characterize the silty (2% sand (2-0.1 μ m), 82 % loess (0.1-0.005 mm), and 16 % clay (< 0.005 mm)) and clayey loess layers (10% sand, 70% loess, and 20 % clay). Based on the particle size distribution curve, 50% of the particles was larger than 1 cm. For this purpose an infiltrometer was installed with filter sections at depths of 5.5 and 9.5 m (see further). The objective of the in-situ test at the second site was to hydraulically characterize the last few meters of the gravelly clay layer (66% sand, 30% loam, and 4% clay), for which a much shorter infiltrometer device was sufficient compared to the first site.

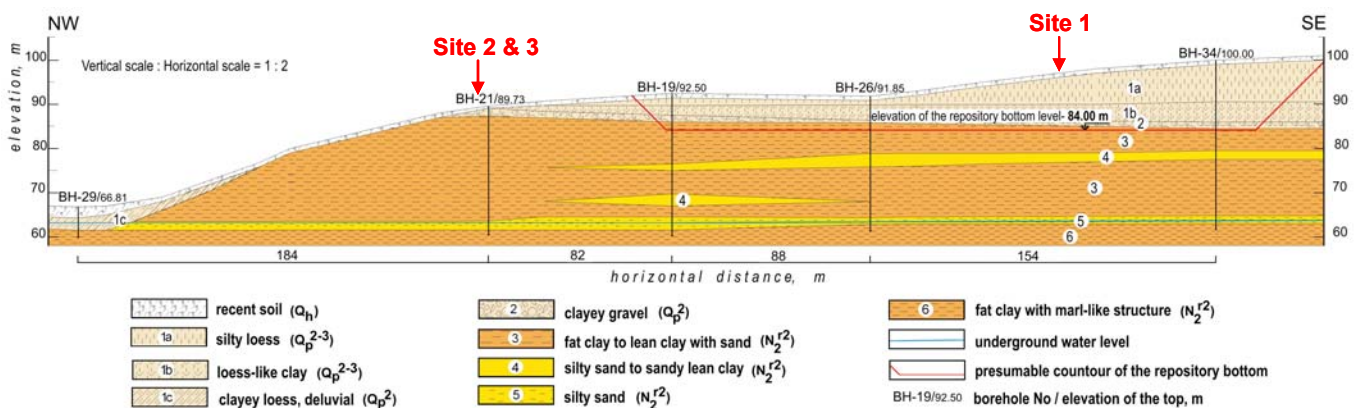


Figure 1 Cross-sectional profile of Marichin Valog site with approximate location of test sites indicated. Infiltrator tests were carried out at Site 1, 2 & 3.

Observed moisture profiles from TRIME measurements

In the framework of the characterization of the unsaturated sediments at the Marichin Valog site, a cylindrical TRIME T3-44 moisture apparatus ([3]; [4]) was used. The TRIME apparatus is based on the Time Domain Reflectometer technique (TDR) ([5]), and should be used together with special polycarbonate access tubes. The TRIME device generates a high-frequency pulse (between 600 MHz and 1.2 GHz) which propagates along the wave guides generating an electromagnetic field around the probe. At the end of the wave guides, the pulse is reflected back to its source. The resulting transit time (10 ps to 2 ns) and dielectric constant are dependent on the moisture content of the medium.

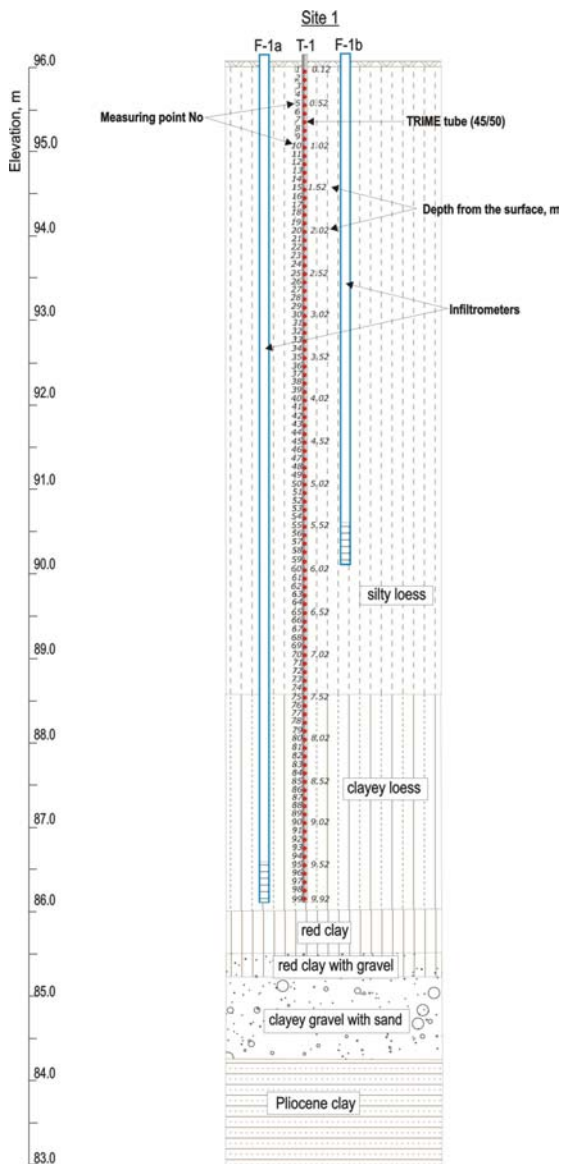


Figure 2 Observation borehole T-1 for water content measurements using TRIME probe, and infiltrimeters F-1a and F-1b. Elevations in m above sea level.

The moisture content was calculated by the TRIME device; we required a custom made calibration because thicker access tubes were used in our experiments compared to the commercially available tubes from IMKO. The TRIME probe has the advantage that one single probe can be used to determine nearly continuous moisture profiles within different access tubes.

Several tubes have been installed at the site, mainly for the purpose of calibration of the probe, for determining time series of moisture profiles, and for carrying out in-situ infiltration tests in undisturbed soil at depths up to 10 m and more. Usually applications with the TRIME apparatus are limited to depths of a few meters ([5]), while in our application the measurement depth is up to 10 m.

TRIME access tubes installed as a component of the infiltrometer set-up have also been used to obtain time series of natural moisture profiles. Details of the access tubes and the measurement depths are shown in Fig. 2. The standard commercial length of access tubes is 3 m. For our purpose, the total length of access tubes was extended until 10 m, using 2-m-long sections with SCK•CEN-made provisions at both ends to allow two neighboring tubes to be smoothly attached and glued together. For the TRIME probe to be useful at those depths, a special extension cable with a maximum length of 21 m was used together with the TRIME IPH module. Until present, moisture profiles have been measured at four different times (see further). A second set of moisture profiles was determined on the basis of undisturbed core samples collected from two boreholes. Careful analysis of these core samples also served for determining a refined stratigraphic description.

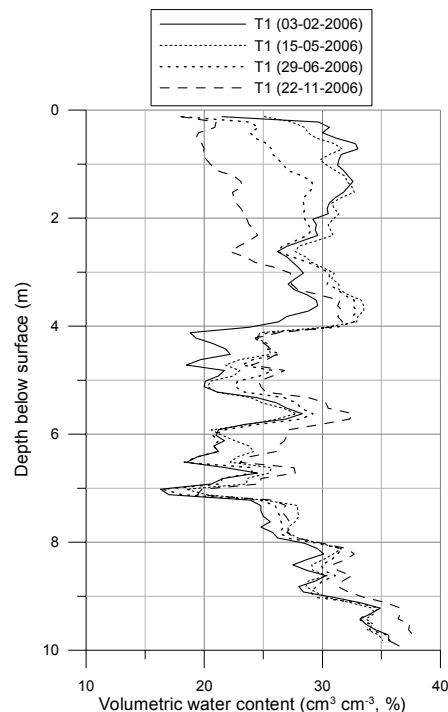


Figure 3 Observed water content based on TRIME readings.

TRIME-based natural water content measurements at different observation times are shown in Fig. 3. For borehole T-1 drying of the profile as time progresses from February 2006 till November 2006 is clearly seen, especially up to depths of 3 m. Deeper in the profile water content variations with time are smaller. For the clayey gravel, average water content increased from 26.6 % at 7.5 m to 36.3 % at 10 m (Fig. 3).

INFILTRMETER SET-UP

At site 1 the deepest infiltrometers were installed at the depths of 5.5 m and 9.5 m (Fig. 2). The first one is located in the silty loess layer, hence is used to determine the hydraulic properties characteristic of the silty loess. The second one is located in the clayey loess, and can be used to determine the hydraulic properties of that layer. Owing to the relatively great depth of the filter sections, much higher constant head values will be applied for infiltrometer 1 compared to the head values used for the less deep filters in site 2.

For the installation of the infiltrometers at site 1, a 150-mm-OD borehole was drilled up to a depth of 6 and 10 m, respectively. The infiltrometer was at 0.5-m distance from the TRIME access tubes (Fig. 2). The infiltrometer consisted of a 75-mm-OD PVC (72-mm-ID) tube with a screened section of 0.5 m at its bottom end (screen started at 7 cm from bottom). Vertically oriented sleeves were made in the PVC to arrange the filter section. After installation of the PVC tube, gravel was poured in the hole until the first meter of the borehole was filled. Then loess from the borehole was poured on the gravel until a layer of 0.7 m loess was obtained. Then bentonite powder was poured in the hole up to a thickness of 0.5 m. Next a 0.5-m-thick concrete layer was made to seal off the filter section. The remaining space until the soil surface was filled with loess from the site. Installation of infiltrometers at the other site was done in the same way.

Each infiltrometer was used as a so-called constant head infiltrometer. Water was injected into the PVC cylinder by means of a flexible tube, to which a heavy metallic weight was attached to keep the end of the flexible tube at a fixed position at the bottom of the cylinder. The flexible tube should be attached to a pump which provides a constant influx of water for the entire duration of the test. The PVC cylinder extended approximately 2 m above the soil surface, where an overflow was provided. In this way a constant water level could be maintained throughout the entire infiltration test.

CONSTANT HEAD INFILTRMETER TESTS: SUMMARY OF DATA AND ANALYSIS

Constant head infiltrometer tests were carried out with infiltrometer F-1a, F-1b, F-2 and F-3. The distance from the different filter sections to the soil surface and the extension was different. As a result, the constant head at the top of the filter section was, respectively 11.4, 7.3, 3.9, and 4.4 m for infiltrometer F-1a, F-1b, F-2, and F-3. Constant head was obtained by supplying water through a flexible tube by means of an adjustable pump. A water level recorder was put in the

infiltrometer tube with the recording depth 1 cm below the level of the overflow. When the water level dropped 1 cm below the overflow level, a signal was given and the pumping rate was increased until the original water level was restored. Such situation did almost not occur during the measurements, since the pumping rate was put slightly larger than the infiltration capacity, with excess water being evacuated through the overflow device, then collected and finally recycled. When steady-state flow conditions were reached, water application was stopped and the infiltration test was finished.

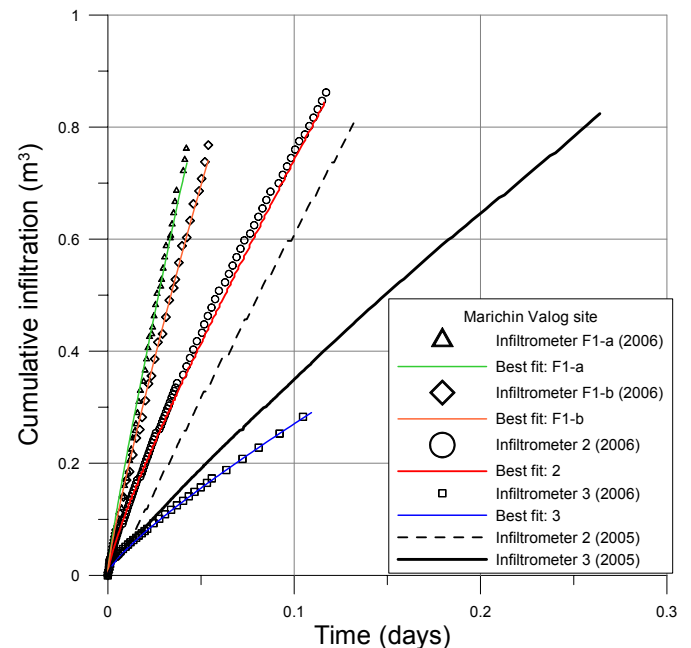


Figure 4 Measured cumulative infiltration for infiltrometer F-1, F-2 and f-3. Best fit simulations using HYDRUS-2D are also included.

Cumulative infiltration for all infiltrometer tests is shown in Fig. 4. In total four tests were carried out in 2006: two tests in the shallow clayey gravel layer (infiltrometer F-2 and F-3), and two tests in deeper loess sediments (F-1a and F-1b) to evaluate the methodology for deep sediments. For the former infiltrometer, initial tests carried out in 2005 were repeated in 2006 to evaluate the reproducibility of such tests.

Different cumulative infiltration was observed for different infiltrometers (Fig. 4). The faster increase in cumulative infiltration for infiltrometer F-1a and F-1b is due in part to the higher imposed heads: approximately 12 m for F-1a and 7 m for F-1b, versus approximately 4.5-5 m for infiltrometer F-2 and F-3. In less than 0.05 days (1.2 hours) a total amount of nearly 0.8 m³ has infiltrated. Approximately twice as much time is needed to infiltrate the same amount for infiltrometer F-2. For infiltrometer 3 a total amount of 0.5 m³ had infiltrated within 0.1 day. For all infiltrometers a steady-state infiltration rate was obtained within the duration of the experiment.

Cumulative infiltration for the 2005 and 2006 tests are different, with the smallest difference being observed for infiltrometer F-2 and largest for infiltrometer F-3. For the former the same slope is observed indicating a very similar infiltration rate (6.55 m³/d in 2006 versus 6.9 m³/d in 2005), while diverging slopes are seen for the latter resulting in slightly different infiltration rates (2.46 m³/d in 2006 versus 3 m³/d in 2005). Taking account of the different initial water content conditions (wetter conditions in 2006), the repeatability of the test is certainly acceptable and the suitability of the test is therefore confirmed.

NUMERICAL MODELING OF CONSTANT HEAD INFILTRMETER TESTS

Inverse estimation of hydraulic properties using borehole infiltration data

The purpose of the in-situ borehole infiltration test is the determination of soil hydraulic functions at a measurement scale that is commensurate with the scale of modelling. The procedure that will be used is outlined below. The parameter estimation by means of numerical inversion is demonstrated using a conceptual model that was specifically developed for the Mariching Valog site ([1],[2]). Initial values for the hydraulic functions that had to be provided for the numerical inversion were estimated on the basis of neural network predictions provided in HYDRUS-2D ([6]). In the predictions we used particle size distribution data as input parameters.

Soil hydraulic properties may be determined by means of inverse optimization techniques such as provided in HYDRUS-2D. Numerical inversion with HYDRUS-2D allows determination of van Genuchten ([7]) soil hydraulic properties (see further) when sufficient and appropriate soil hydraulic data is measured, e.g. during constant head infiltration in a borehole when cumulative infiltration and history of water content in the undisturbed sediment at several locations are measured.

For our applications, inverse optimization comprises computer simulation of 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. The simulation starts with "guess" or "trial" values of the soil hydraulic properties; these values may be estimated using neural network predictions based on particle size data, or by using some other prior information, such as the optimized values from laboratory testing ([1]). In the optimization hydraulic properties are gradually changed until the calculated cumulative infiltration and soil moisture profile agrees well with the measurements.

Application of the inverse optimization required developing an axisymmetric model in HYDRUS-2D for each of the four infiltrometers. The vertical dimension of the model was limited to the soil layers that would be immediately influenced by the infiltrating water. The lateral dimension of the model was sufficiently large such that lateral boundary conditions would not influence the simulation results.

Water flow through the unsaturated sediments was described by means of the van Genuchten water retention characteristic, or water retention curve, $\theta(h)$, defined as ([7]):

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

where θ is water content (cm³/cm³), h is matric head (m), θ_r and θ_s are residual and saturated water content (cm³/cm³), respectively, and α (1/m), n , and m are constants which define the shape of the curve, with $m = 1 - 1/n$ (with the requirement $n > 1$ if Eq. 1 is used in combination with $K(h)$).

In addition to the parameterisation of $\theta(h)$, description of water flow through unsaturated soil also requires the parameterisation of the unsaturated hydraulic conductivity $K(h)$. Most models for $K(h)$ assume that the water-filled pore space consists of a set of capillaries with the distribution of pore radii being determined by the soil water characteristic. One very attractive unsaturated hydraulic conductivity function is that derived by van Genuchten ([1]), and is based on the statistical pore size distribution of ([8]). The van Genuchten-Mualem $K(h)$ model is defined as follows:

$$K(h) = \begin{cases} K_s K_r(h) & h < 0 \\ K_s & h \geq 0 \end{cases} \quad (2)$$

where

$$K_r = S_e^\tau [1 - (1 - S_e^{1/m})^m]^2 \quad (3)$$

and K_s and K_r are saturated and relative hydraulic conductivity (m/s), respectively, τ is an empirical constant assumed equal to 0.5 ([8]), and S_e is saturation degree, defined as:

$$S_e = \frac{\theta - \theta_r}{\theta_s - \theta_r} \quad (4)$$

where θ is soil water content (cm³/cm³), θ_r and θ_s are the residual and saturated water contents (cm³/cm³), respectively. As a first approximation and on intuitive ground, $\theta_s = \eta$ (total porosity) and $\theta_r = 0$. In reality, however, the saturated water content θ_s of field soils is generally 5 to 10% smaller than the total porosity η because of entrapped air and the presence of large pores which drain too rapidly to become saturated ([9]). The residual water content θ_r is likely to be larger than zero, because of the presence of adsorbed water. Furthermore, the residual water content is an extrapolated parameter, and may therefore not necessarily represent the smallest possible water content in a soil. Most often θ_r is treated as a fitting parameter without physical significance ([9]).

The advantage of the van Genuchten-Mualem $K(h)$ model is that nearly all its parameters, except K_s , can be determined from the soil water characteristic. In other words, a complete description of $\theta(h)$ and $K(h)$ may be obtained with four parameters, i.e. θ_r , θ_s , α , n , and one additional parameter, K_s .

In the optimization of the $\theta(h)$ and $K(h)$ relationships, the θ_r and θ_s parameters were fixed to decrease the degrees of freedom and to reduce problems of non-uniqueness in the optimization. Parameter θ_s was put equal to total porosity while θ_r was fixed at 0.05.

The automatic parameter optimization routine provided in HYDRUS-2D was invoked to further optimize the parameters α and K_s . HYDRUS adopts the minimization of the sum of the squares (SSQ) of the residuals:

$$SSQ = \sum_{i=1}^N (q_{p,i} - q_{o,i})^2 \quad (5)$$

where N is the number of calibration points (here only the cumulative fluxes are used), $q_{p,i}$ is the i th predicted values, and $q_{o,i}$ is the i th observed value. HYDRUS uses the Marquardt-Levenberg optimization algorithm to minimize the objective function (Eq. 5), to come up with parameters that produce the minimum difference between the observed and predicted values. In the optimization the parameter n was excluded from being optimized because initial calculations where n was included showed high correlation with parameters α and K_s , and a high standard error coefficient for n indicative of non-uniqueness of the solution. The parameter n was therefore kept constant and equal to 2 [2].

Results from inverse optimization

Results from parameter optimization for infiltrometer F1-a are summarized in Table 1. Since the filter section of F1-a is in contact with clayey loess material, parameters for this layer were determined first. Best fit values for α and K_s with a low standard error (SE) coefficient were obtained for the clayey loess. After five iterations the SSQ did not further decrease (true for all infiltrometers). A comparison between observed and calculated cumulative infiltration is given in Fig. 4.

Table 1 Parameter values from inverse optimization using HYDRUS-2D (infiltrometer F1-b, silty loess). Parameter n was fixed at 2.

Parameter	Best fit value	S.E. coefficient	Lower 95%	Upper 95%
α (1/m)	0,0586	0,00849	0,04177	0,0754
K_s (m/day)	0,0449	0,00068	0,0436	0,0463
SSQ	0,00281			
R^2	0,99939			

Optimized parameter values for infiltrometer F1-b are given in Table 1, illustrating again a very good fit, with acceptable SE coefficients. Other parameters (n , θ_r , and θ_s) were fixed during the optimization, with $\theta_s = 0.44$, the independently derived total porosity ([1]). Further comparison between observed and fitted cumulative infiltration is given in Fig. 4.

Results for infiltrometer 2 whose filter section was placed in the clayey gravel are summarized in Table 2. A much higher α value was obtained compared to infiltrometer F1-a. This

observation is in agreement with the general soil physical concept that coarser materials have larger α -values ([10]). For this material the saturated water content, θ_s , was also fitted, since no estimates of total porosity were available. The fitting of θ_s was done only after α and K_s were fitted, and the latter two parameters were kept fixed at their optimal value while fitting θ_s . Fitting of all three parameters together resulted in non-uniqueness in the solution. A graphical comparison between observed and calculated cumulative infiltration is given in Fig. 4.

Table 2 Parameter values from inverse optimization using HYDRUS-2D (infiltrometer F-2, clayey gravel). Parameter n was fixed at 2, while $\theta_r = 0.05$ and $\theta_s =$ fitted. Values in square brackets from 2005 campaign ([1]).

Parameter	Best fit value	S.E. coefficient	Lower 95%	Upper 95%
α (1/m)	3 [0,53]	1.167	0,7014	5,298
K_s (m/day)	0,09125 [0,041]	0,000739	0,089	0,0927
θ_s	0,413 [#]	0,00011	0,411	0,416
SSQ	0,00251 (0,000605) [#]			
R^2	0,99935 (0,99940) [#]			

[#] when θ_s fitted separately

CONCLUSIONS

The Marichin Valog site located in the vicinity of Kozloduy NPP is considered by the State Enterprise Radioactive Waste (SE-RAW) a potential site for final disposal of low-and intermediate level short-lived radioactive waste. To prepare for an in-depth evaluation of the suitability of the Marichin Valog site, site characterization was carried out in 2005 and 2006 by the Geological Institute of the Bulgarian Academy of Sciences and SCK•CEN emphasizing on determination of the unsaturated flow characteristics of the unsaturated geological materials. Over the past two years, the hydraulic characteristics of the variably saturated Quaternary sediments (a sequence of silty and clayey loess, red clay and clayey gravel) at the Marichin Valog experimental site have been determined by means of laboratory and field tests. The present document reports results from the constant head infiltrometer field tests carried out in 2005 and 2006.

The objective of in-situ field tests was to evaluate the feasibility of the infiltrometer set-up for several unsaturated layers with varying depths below soil surface. For this purpose four infiltrometer tests were carried out. The first two to confirm earlier results for infiltrometers installed up to the depth of 3 m in very heterogeneous clay layer mixed with gravel or carbonate concretions. The second two to test the technique in clayey and silty loess at depths up to 10 m.

Testing the repeatability of the infiltrometer test by comparing results from 2005 and 2006 was partly successful. Estimated saturated hydraulic conductivity values for one and the same infiltrometer were in good agreement. The 2006 shape-curve parameters α were not in good agreement with the

2005 values. Possibly the sampling of a different part of the soil material surrounding the infiltrometer could have caused this difference, in combination with large spatial variability.

Results from the two deeper infiltration tests in clayey loess and silty loess were satisfactory: steady-state flow was obtained within a reasonable short period (i.e., less than 0.1 day), and no technical difficulties were observed. Cumulative infiltration curves could be fitted well with similar unsaturated parameters, although the much lower content of large-sized particles such as gravel and carbonate concretions resulted in much lower α -values more typical of loess or loam material. Difference in saturated hydraulic conductivity between different materials was relatively small, i.e. less than a factor of five between minimal and maximum value.

One of the most difficult to characterize layers was the clayey gravel and carbonate rich layer. Owing to the large-sized concretions and gravels, laboratory determination of hydraulic properties is nearly impossible, leaving only field-determination as a viable option. The use of borehole infiltration data in the inverse optimization routine of the computer code HYDRUS-2D is a practical and reliable methodology to obtain such field-scale hydraulic properties.

The innovative features of our approach comprise use of constant-head infiltrometers at relatively great depth below surface whereby in combination advancing water fronts are monitored by means of cylindrical TRIME TDR probes and volumes of water infiltrated. All data may be integrated in the parameter optimization routine of HYDRUS-2D for inverse optimization of hydraulic parameters.

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