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 convection-dispersion 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 one-dimensional form is given as follows:

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

(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 \( K(h) \):

\[
\begin{align*}
\theta(h) &= \begin{cases} 
\theta_s + \frac{\theta_s - \theta_r}{\left(1 + \alpha|h|\right)^m} & h < 0 \\
\theta_r & h \geq 0
\end{cases} \\
K(h) &= \begin{cases} 
K_s K_r(h) & h < 0 \\
K_s & h \geq 0
\end{cases}
\end{align*}
\]

(2)

(3)

where
\[ K_r = S_e \left[ 1 - \left(1 - S_e^{1/m}\right)^m \right]^2 \]  

(4)

and where \( \theta_r \) and \( \theta_s \) are, respectively, the residual and saturated water contents [L\(^3\)L\(^{-3}\)], \( \alpha \) [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:

\[
S_e = \frac{\theta - \theta_r}{\theta_s - \theta_r}
\]

(5)

According to the van Genuchten-Mualem model, knowledge of the five parameters \( \theta_s \), \( \theta_r \), \( \alpha \), \( n \), 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 \( \theta_s \), \( \theta_r \), \( \alpha \), 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.

<table>
<thead>
<tr>
<th>Soil description</th>
<th>Parameter</th>
<th>Best fitted value</th>
<th>S.E. coefficient</th>
<th>Lower 95%</th>
<th>Upper 95%</th>
</tr>
</thead>
<tbody>
<tr>
<td>Clayey loess*</td>
<td>$\alpha$ [m$^{-1}$]</td>
<td>0.351</td>
<td>0.0354</td>
<td>0.281</td>
<td>0.490</td>
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<tr>
<td></td>
<td>$K_s$ [m$^{-1}$s$^{-1}$]</td>
<td>6.03E-07</td>
<td>0.00144</td>
<td>0.0492</td>
<td>0.0549</td>
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<tr>
<td></td>
<td>SSQ</td>
<td>0.0119</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>$R^2$</td>
<td>0.997</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Red clay</td>
<td>$\alpha$ [m$^{-1}$]</td>
<td>0.497</td>
<td>0.450</td>
<td>-3.395</td>
<td>1.39</td>
</tr>
<tr>
<td></td>
<td>$n$ [-]</td>
<td>4.29</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>$K_s$ [m$^{-1}$s$^{-1}$]</td>
<td>6.89E-07</td>
<td>0.0229</td>
<td>0.0140</td>
<td>0.105</td>
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<tr>
<td></td>
<td>SSQ</td>
<td>0.0118</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>$R^2$</td>
<td>0.997</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Silty loess*</td>
<td>$\alpha$ [m$^{-1}$]</td>
<td>0.0586</td>
<td>0.00849</td>
<td>0.0418</td>
<td>0.0754</td>
</tr>
<tr>
<td></td>
<td>$K_s$ [m$^{-1}$s$^{-1}$]</td>
<td>5.20E-07</td>
<td>0.00068</td>
<td>0.0436</td>
<td>0.0463</td>
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<tr>
<td></td>
<td>SSQ</td>
<td>0.00281</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>$R^2$</td>
<td>0.999</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Clayey gravel*</td>
<td>$\alpha$ [m$^{-1}$]</td>
<td>3.00</td>
<td>1.17</td>
<td>0.701</td>
<td>5.30</td>
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<tr>
<td></td>
<td>$K_s$ [m$^{-1}$s$^{-1}$]</td>
<td>1.06E-06</td>
<td>0.000739</td>
<td>0.0989</td>
<td>0.0927</td>
</tr>
<tr>
<td></td>
<td>$\theta_i$ [cm$^3$cm$^{-3}$] **</td>
<td>0.431</td>
<td>0.00011</td>
<td>0.411</td>
<td>0.416</td>
</tr>
<tr>
<td></td>
<td>SSQ</td>
<td>0.00251</td>
<td>(0.000605)**</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>$R^2$</td>
<td>0.999 (0.999)**</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Highly carbonated zone*</td>
<td>$\alpha$ [m$^{-1}$]</td>
<td>2.68</td>
<td>2.29</td>
<td>-1.85</td>
<td>7.21</td>
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<tr>
<td></td>
<td>$K_s$ [m$^{-1}$s$^{-1}$]</td>
<td>1.88E-07</td>
<td>0.000246</td>
<td>0.0158</td>
<td>0.0168</td>
</tr>
<tr>
<td></td>
<td>$\theta_i$ [cm$^3$cm$^{-3}$] **</td>
<td>0.354</td>
<td>0.0229</td>
<td>0.308</td>
<td>0.399</td>
</tr>
<tr>
<td></td>
<td>SSQ</td>
<td>0.00391</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>$R^2$</td>
<td>0.998</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

*Parameter $n$ is fixed at 2; ** when $\theta_i$ 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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