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A new method to estimate the parameters of van Genuchten retention model using degree of phosphorus saturation (DPS)

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Soil water retention curve is necessary for many studies of water and solute transport in soils. Among the developed mathematical models, one of the most widely used models to describe the water-retention curve of soils is van Genuchten model. Its four parameters are the key to application of this model. In this study we introduced in detail the parameter estimation procedure of the model using DPS system based on the retention data (namely soil water suctions and corresponding soil water contents for cinnamon soil in northeastern China), and obtained the values of the four parameters. The water content values calculated by established model and the measured values were analyzed with the methods of variance analysis and residual analysis. The results showed that the nonlinear regression model had good estimate effects, and the relationship between estimated and observed values was significant at to 0.0001 levels. Additionally, the root mean square residual (RMSR) between measured and estimated water contents was less than 0.008 cm³ cm⁻³ and the absolute values of relative error of soil water contents was in the range of 0.05 to 7.0%. Although the estimated parameter values of van Genuchten model using DPS had the same precision as those estimated with MATLAB, the efficiency and universality was improved obviously as compared to those using MATLAB. Therefore, this method is practical and feasible to obtain values of four parameters of van Genuchten model for soil scientists.

Key words: Soil water retention curve, van Genuchten model, degree of phosphorus saturation (DPS) system.

INTRODUCTION

Soil water retention curve (SWRC) is a basic hydrophysical characteristic of soil, described as the dependence between soil water content and soil water potential. A detailed knowledge of soil water potential-soil water content characteristics is important to simulate the transport of water and contaminants in soils. Different models to describe the soil water retention characteristics are available and have been evaluated by many scholars (Alexander and Skaggs, 1986; Leij et al., 1997; Christen et al., 2006). Among the developed empirical models, van Genuchten model (1980) historically has been widely adopted because of a higher degree of fitting to observed soil retention data, especially for undisturbed and many fine-textured soils. However, a key to practical application of this model is how to obtain the four unknown parameters on the base of known experimental data (namely measured soil water suctions and corresponding soil water contents). This is the reason that we are frequently confronted with situations where some problems related to convergence and parameter uniqueness remain to be solved when van Genuchten retention model is estimated by traditional least square method from water retention data. Another reason is that van Genuchten model exhibits highly nonlinear characteristics. So, many attempts have been done to develop indirect methods, which enable soil water retention model by van Genuchten (1980) to be determined based on the soil physical properties (for example, particle-size distributions, organic matter content and bulk density) routinely measured in laboratories (Arya et al., 1999a; Schaap et al., 2001; Walczak et al., 2002; Christen et al., 2006; Ghanbarian-Alavijeh et al.,

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Whereas in simulations of water and solute transport at plot, field and large scale (region, catchment) it is often not possible to parameterise the models representing different soil types, due to lack of detailed soil physical properties.

As far as our country is concerned, some researchers also cost a lot of time and labour to explore available methods to estimate the parameters of van Genuchten model. Shao et al. (2000a, b) presented a simple infiltration method for determining the parameters of water retention model proposed by van Genuchten (1980) based on the Richards’ equation for one-dimensional soil water movement. Wang et al. (2000) combined the least square method with non-linear simplex approach to calculate the parameters of van Genuchten model from water retention data. Xu et al. (2000) subsequently developed a numerical technique for solving the $\theta(h)$-based form of the van Genuchten model in a sandy loamy soil by means of least square method coupled with Picard iteration approach. Additionally, several others (Li et al., 2001; Wei et al., 2004) also estimated van Genuchten SWRC of unsaturated soils using the parameter optimization method with the simplex algorithm or the RETC (retention curve) code (van Genuchten et al., 1991). Recently, Wei et al. (2004) estimated the four parameters of van Genuchten model for cinnamon soil by MATLAB (matrix laboratory) software (Su and Ruan, 2002). This undoubtedly produced a very accurate method for obtaining the SWRC parameters, and successfully solved the problem involving the high nonlinearity of van Genuchten model. Although these methods mentioned earlier have obtained good agreement with the experimental results, unfortunately they have to be done either through the various infiltration experiments in soil column (Bohne et al., 1992; Šimůnek and van Genuchten, 1996; Schwartz and Evett, 2003; Steenpass et al., 2010), computer programming (van Genuchten et al., 1991; Warrick, 1992; Schaap et al., 2001; Hodnett and Tomasella, 2002; Ma et al., 2005; Šimůnek et al., 2008;) or possibly through the use of special software (Kool et al.,1987; Vrugt et al., 2008a, b). Thus, most of the current methods remain relatively time-consuming, costly, and low efficiency, and which are often subjected to limitations in practical applications.

MATLAB is a kind of computing software with great convenience and strong function, but the researchers in China are often hampered and cannot adapt themselves to its operating interface because of the requirements of very specific mathematic knowledge and/or good abilities in English and programming.

To a certain extent, this would directly restrict its use in the field of domestic soil physics. Consequently, it is necessary to provide a universal and rapid method to determine unknown parameters in van Genuchten retention model of unsaturated soil and satisfy the demand of researchers as far as possible, who are weak in mathematics or programming. The objectives of this study are therefore:

1. To provide the readers a simple and rapid method about parameter estimation of van Genuchten model through Data Processing System (DPS).
2. To analyze the feasibility of parameter estimation and compare parameters of van Genuchten retention model obtained by DPS with estimated parameters obtained from Wei et al. (2004) by MATLAB.

MATERIALS AND METHODS

Model description

The van Genuchten water retention model used for this study is described as:

$$
\theta(h) = \theta_s + \frac{\theta_r - \theta_s}{1 + \left(\frac{h}{\alpha}\right)^m}
$$

(1)

Where $\theta(h)$ is the actual soil water content (cm$^3$cm$^{-3}$) at the suction $h$ (cm), taken positive for increasing suctions; $\theta_r$ and $\theta_s$ are the residual and saturated soil water contents (cm$^3$cm$^{-3}$), respectively; $\alpha$ is a parameter related to the inverse of the air entry suction (cm$^3$); $m$ and $n$ are curve shape parameters (van Genuchten, 1980). Note that $m$ here characterizes the asymmetry using the constraint $m=1$/$n$, therefore the water retention characteristics defined by Equation (1) only contain four unknown parameters, that is, $\theta_r$, $\theta_s$, $\alpha$, and $n$.

Data source

As an illustrative example, we selected here a set of water retention data measured by Wei et al. (2004) during September 2004 from a field test site in northeast China to estimate van Genuchten model parameters. The eight point data on the water retention curve for the cinnamon soil whose texture is clay were listed in Table 1.

Parameter estimation procedure

DPS developed by Tang and Feng (2002, 2007) is a multipurpose processing platform with statistical analysis, numerical computation, and mathematical models, etc. Now this system has been developed to version 12.01. One of the most important features of DPS is that it allows user friendly access to operating interface, which consists of two menu-controlled and easy to understand windows (Figure 1). The first window (spreadsheet window), in which input data can be entered manually or as a formatted EXCEL file, provides general database information (for example, number of records in the database) and output results. Input and output data are stored in various sheets in the same database file. The second window (text editing window) serves to make estimations of the four parameters in van Genuchten model whose mathematical expression can be edited using near natural languages. Especially, more information about various aspects of DPS may be obtained through the help system which can be accessed from anywhere within this software. Therefore, DPS can make it easy to solve complicated nonlinear models, which are extremely hard to solve or even cannot be solved in the past. In this study, we estimated water retention parameters of van Genuchten model by DPS in conjunction with Levenberg-Marquardt method (Marquardt, 1963).
Table 1. Soil water suctions and soil water contents for cinnamon soil in China.

<table>
<thead>
<tr>
<th>SWS (cm)</th>
<th>0.00</th>
<th>50.65</th>
<th>293.77</th>
<th>790.14</th>
<th>992.74</th>
<th>5065.00</th>
<th>10130.00</th>
<th>15195.00</th>
</tr>
</thead>
<tbody>
<tr>
<td>SWC(cm$^3$m$^{-3}$)</td>
<td>0.5650</td>
<td>0.4013</td>
<td>0.2502</td>
<td>0.2324</td>
<td>0.2307</td>
<td>0.1926</td>
<td>0.1812</td>
<td>0.1730</td>
</tr>
</tbody>
</table>

The SWS and SWC represent soil water suction and soil water content, respectively.

Figure 1. Data input and formula definition in DPS system.

combined direct solution and the steepest descent approach. The parameter values were determined by minimizing the objective function according to:

$$Q(P) = \sum_{i=1}^{N} \left( \theta_i - \theta_i^* \right)^2$$

(2)

Where $\theta_i$ and $\theta_i^*$ are the measured and estimated water contents, respectively. $N$ is the number of measured water retention points for soil sample and $P$ is the parameter vector ($\theta$, $\theta_s$, $\alpha$, $n$). The procedure involves several steps.

The first step was to input and edit data in an electronic sheet of DPS system. Namely, a row denotes a sample, and a column shows a variable. The unanalyzed data are then defined as a data block where the first column is variable $x_1$, the second one is variable $x_2$ and the third variable $x_3$, and so on. These variables above are ranged in order where an independent variable must appear ahead of a dependent variable. Accordingly, the data in
The water content values for the cinnamon soil, calculated using the van Genuchten water-retention curve determined by DPS have been compared with the water content values measured. The comparison was done by the residual analysis between measured and calculated soil water contents (Table 3). The retention parameter values and the RMSR were presented to the two adopted methods for DPS and MATLAB (Table 4). From Table 3 it can be known that the established model (Equation 4) estimated moisture content, at different soil water suction values, with good accuracy. This is confirmed by very small values of the residual squares and the relative errors derived from DPS, respectively. This is seen that the range of relative error is below 5% (except the water content at 293.77 cm suction), similarly as the results of MATLAB (Table 3). Meanwhile we found that the RMSR values are 0.0077 cm$^{-3}$ for DPS and 0.0078 cm$^{-3}$ for MATLAB respectively, both of which are less than 0.008 cm$^{-3}$ (Table 4). That is to say, the water contents estimated by DPS and MATLAB are extremely close to the measured values, which supported well the findings of variance analysis above. Compared with the results obtained with MATLAB originally proposed by Wei et al. (2004), we found only a
Figure 2. The results of parameter estimation for van Genuchten model.

The results of parameter estimation for van Genuchten model are presented in the table. The DPS method shows minor improvement (lower RMSR) in the parameter estimation using DPS, but the lower RMSR indicated that DPS method gave this model a higher degree of flexibility in fitting to retention data for the clayey soil. This showed that the DPS method is reasonable and reliable to estimate the four parameters of van Genuchten water retention model.

Conclusions

This study presents the DPS which implements a new procedure for estimation of water retention parameters as well as associated accuracy test. In this process of the parameter estimation for van Genuchten model, here the complex mathematical symbols and the complicated
Table 2. Variance analysis of van Genuchten model for water retention.

<table>
<thead>
<tr>
<th>Method</th>
<th>Source</th>
<th>Sum of squares</th>
<th>d.f.</th>
<th>Mean square</th>
<th>F test</th>
<th>P-value</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>DPS</td>
<td>Regression</td>
<td>0.1299</td>
<td>3</td>
<td>0.0433</td>
<td>363.22</td>
<td>0.0001</td>
</tr>
<tr>
<td></td>
<td>Residual</td>
<td>0.0005</td>
<td>4</td>
<td>0.0001</td>
<td>253.13</td>
<td>5.1389E-5</td>
</tr>
<tr>
<td></td>
<td>Total</td>
<td>0.1304</td>
<td>7</td>
<td>0.0186</td>
<td></td>
<td></td>
</tr>
<tr>
<td>MATLAB</td>
<td>Regression</td>
<td>0.1297</td>
<td>3</td>
<td>0.0432</td>
<td>253.13</td>
<td>5.1389E-5</td>
</tr>
<tr>
<td></td>
<td>Residual</td>
<td>0.0007</td>
<td>4</td>
<td>0.0002</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Total</td>
<td>0.1304</td>
<td>7</td>
<td>0.0186</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table 3. Residual analysis of van Genuchten retention model for cinnamon soil.

<table>
<thead>
<tr>
<th>SWS (cm)</th>
<th>Soil water content (cm$^3$ cm$^{-3}$)</th>
<th>Residue (cm$^3$ cm$^{-3}$)</th>
<th>Residual square (cm$^3$ cm$^{-3}$)</th>
<th>Relative error (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Measured</td>
<td>Calculated</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.00</td>
<td>0.5650</td>
<td>0.5653(0.5652)</td>
<td>-0.0003(0.0002)</td>
<td>9.0E-8(4.0E-8)</td>
</tr>
<tr>
<td>50.65</td>
<td>0.4013</td>
<td>0.3983(0.3970)</td>
<td>0.0030(-0.0043)</td>
<td>9.0E-6(1.8E-5)</td>
</tr>
<tr>
<td>293.77</td>
<td>0.2502</td>
<td>0.2656(0.2675)</td>
<td>-0.0154(0.0173)</td>
<td>2.4E-4(3.0E-4)</td>
</tr>
<tr>
<td>790.14</td>
<td>0.2324</td>
<td>0.2259(0.2274)</td>
<td>0.0065(-0.0050)</td>
<td>4.2E-5(2.5E-5)</td>
</tr>
<tr>
<td>992.74</td>
<td>0.2307</td>
<td>0.2193(0.2206)</td>
<td>0.0114(-0.0101)</td>
<td>1.3E-4(1.0E-4)</td>
</tr>
<tr>
<td>5065.0</td>
<td>0.1926</td>
<td>0.1894(0.1891)</td>
<td>0.0032(-0.0035)</td>
<td>1.0E-5(1.2E-5)</td>
</tr>
<tr>
<td>10310</td>
<td>0.1812</td>
<td>0.1827(0.1818)</td>
<td>-0.0015(0.0006)</td>
<td>2.3E-6(3.4E-7)</td>
</tr>
<tr>
<td>15195</td>
<td>0.1730</td>
<td>0.1798(0.1785)</td>
<td>-0.0068(0.0055)</td>
<td>4.6E-5(3.1E-5)</td>
</tr>
</tbody>
</table>

The data in the parentheses were sourced from Wei et al. (2004).

Table 4. Estimated parameters of the van Genuchten retention model for cinnamon soil.

<table>
<thead>
<tr>
<th>Method</th>
<th>$\theta_r$ (cm$^3$ cm$^{-3}$)</th>
<th>$\theta_s$ (cm$^3$ cm$^{-3}$)</th>
<th>$\alpha$ (cm$^{-1}$)</th>
<th>n</th>
<th>RMSR(cm$^3$ cm$^{-3}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>DPS</td>
<td>0.1676</td>
<td>0.5653</td>
<td>0.0475</td>
<td>1.5293</td>
<td>0.0077</td>
</tr>
<tr>
<td>MATLAB</td>
<td>0.1641</td>
<td>0.5652</td>
<td>0.0506</td>
<td>1.5003</td>
<td>0.0078</td>
</tr>
</tbody>
</table>

The $\theta_r$ and $\theta_s$ represents the residual volumetric water contents and saturated volumetric water contents, respectively. The $\alpha$ and $n$ indicates the parameter related to the inverse of the air entry suction and curve shape parameter, respectively.

mathematical deduction are not required. This method, which has the advantages of simplicity of operation, rapid solving and readability over existing methods, really makes solving complex mathematical problems faster and easier, just “what you want is what you see, what you see is what you get”.

On the basis of the eight water content-suction pairs, the DPS successfully solved the four unknown parameters of van Genuchten model using the Levenberg-Marquardt algorithm so as to minimize the sum of squared residuals. According to the variance analysis and significance test of the nonlinear regression, the estimated parameter values reached the extremely significant level ($p = 0.0001$), while the regression coefficient was close to 1. Established the van Genuchten retention model to the retention data gave the RMSR of 0.0077 cm$^3$cm$^{-3}$ and the relative error range of -4.0 to 7.0%. These results suggest that the parameter estimation of van Genuchten model with DPS has the same higher precision as that estimated with MATLAB in the literature (Wei et al., 2004). From the view of practical application, however, the DPS can not only improve the commonality obviously, but also save time and enhance effectiveness greatly, compared with the MATLAB. Therefore, a simple and handy method to estimate the parameters with the numerical computation through DPS was provided for scientists who are engaged in pedology research.

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