Development of pedotransfer functions for soil hydraulic properties in the critical zone on the Loess Plateau, China

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Abstract

Soil hydraulic properties (SHPs) including the soil water retention curve and saturated soil hydraulic conductivity ($K_s$) are crucial input data for simulations of soil water and solute transport in the Earth’s critical zone. However, obtaining direct measurements of SHPs at a wide range of scales is time consuming and expensive. Pedotransfer functions (PTFs) are employed as an alternative method for indirectly estimating these parameters based on readily measured soil properties. However, PTFs for SHPs for the deep soil layer in the Earth’s critical zone are lacking. In this study, we developed new PTFs in the deep soil profile for $K_s$ and soil water retention curve on the Loess Plateau, China, which were fitted with the van Genuchten equation. In total, 206 data sets comprising the hydraulic and basic soil properties were obtained from three typical sites. Samples were collected from the top of the soil profile to the bedrock by soil core drilling. PTFs were developed between the SHPs and basic soil properties using stepwise multiple linear regression. The PTFs obtained the best predictions for $K_s$ ($R_{adj}^2 = 0.561$) and the worst for van Genuchten $\alpha$ ($R_{adj}^2 = 0.474$). The bulk density and sand content were important input variables for predicting $K_s$, $\alpha$, and $\theta_s$, and bulk density, clay content, and soil organic carbon were important for $n$. The PTFs developed in this study performed better than existing PTFs. This study contains the first set of PTFs of SHPs to be developed for the deep profile on the Loess Plateau, and they may be applicable to other regions.

KEYWORDS

Earth’s critical zone, Loess Plateau, pedotransfer functions, soil hydraulic properties

1 | INTRODUCTION

The Earth’s critical zone (ECZ) is located from the top of the plant canopy vertically down to the weathered bedrock and is a key area for sustaining ecosystem function and human survival (Lin, 2010). The water cycle comprises the core process that links the cycling of materials in the ECZ. Hydrological models of soil water dynamics are effective tools for studying the water cycle in the ECZ. Soil hydraulic properties (SHPs), which include the soil water retention curve (SWRC) and saturated soil hydraulic conductivity ($K_s$), are important input parameters for hydrological models. However, obtaining direct measurements of SHPs is expensive, time consuming, and labour-intensive. Thus, an efficient pedotransfer function (PTF) is necessary for producing reasonably accurate estimations of SHPs by using the basic soil properties as inputs and obtaining the hydraulic parameters as outputs (Bouma, 1989).

In recent decades, many PTFs have been developed for SHPs at different scales using various methods (Li, Chen, White, Zhu, & Zhang, 2007; Santra & Das, 2008; Schaap, Leij, & Genuchten, 2001; Wösten, Pachepsky, & Rawls, 2001; Yao et al., 2015). For example, Vereecken, Maes, Feyen, and Darius (1989) sampled the soil horizons in 40 important Belgian soil series and estimated the soil moisture retention characteristics based on the texture, bulk density (BD), and carbon content using nonlinear regression analysis. Wösten, Lilly, Nemes, and Bas (1999) developed PTFs for SHPs by using a database of the hydraulic properties of European soils (HYPRES) by multiple regression analysis.

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Schaap et al. (2001) presented a computer program (ROSETTA) based on neural network analyses for estimating the SWRC and $K_s$ for soils in the United States. Li et al. (2007) used multiple linear regression analysis to estimate the SHPs of Fengqiu County soils on the North China Plain. Wang, Shao, and Liu (2012) predicted the SHPs for the Chinese Loess Plateau based on multiple linear regression equations, and Zhao, Shao, Jia, Nasir, and Zhang (2016) also used PTFs to estimate the soil hydraulic conductivity on the Loess Plateau of China by multiple linear regression and artificial neural networks. However, it should be noted that the previously developed PTFs for SHPs were mainly for upper soil layers (of depths < 3 m), and no studies have considered the PTFs for deep layers in the ECZ.

The Loess Plateau area of China is predominantly covered by loessial deposits with thicknesses ranging from 50 to 200 m, and two thirds of this area contains arid and semi-arid regions. Thus, there is a need for reliable SHPs data to study the hydraulic processes that occur in the ECZ. However, it is difficult to obtain direct measurements of SHPs in deep soil profiles. Therefore, PTFs should be developed to obtain indirect estimates of the SHPs for deep soil profiles on the Loess Plateau.

Therefore, the objectives of the present study were (a) to characterize descriptive statistics for the SHPs of soil material at various depths on the Loess Plateau, (b) to develop PTFs for the SHPs in the ECZ on the Loess Plateau, and (c) to compare the results obtained using these new PTFs with those produced by existing PTFs.

2 | MATERIALS AND METHODS

2.1 | Study area description

The study was conducted across the entire Loess Plateau of China ($33^\circ 43′$–$41^\circ 16′$ N, $100^\circ 54′$–$114^\circ 33′$ E), which is located in the continental monsoon climate region and covers approximately 6.5% of China (Figure 1a). The annual precipitation ranges from 150 mm in the northwest to 800 mm in the southeast, where 55–78% falls from June to September (Shi & Shao, 2000). The annual solar radiation ranges from $5.0 \times 10^9$ to $6.7 \times 10^9$ J m$^{-2}$. The annual evaporation on the Loess Plateau is 1,400–2,000 mm, and the mean annual temperature ranges from 3.6°C in the northwest to 14.3°C in the southeast (Shi & Shao, 2000). The region is surrounded by mountains, where the loessial landforms include Yuan (a large flat surface with little erosion), ridges, hills, and gullies.

2.2 | Soil sampling

Three typical sampling sites (Yangling, Changwu, and An'sai; Figure 1b) were selected from south to north on the Loess Plateau, and soil samples were collected from the soil surface to the bedrock using drilling equipment (assembled by Xi’an Qinyan Drilling Co. Ltd). At each sampling site, metal cylinders (diameter: 5 cm, length: 5 cm) were used to collect undisturbed soil samples from the midpoint of each 1-m interval of the soil boring (0.5, 1.5, 2.5, and 3.5 m ..) to obtain measurements of $K_s$, SWRC, and BD. Similarly, disturbed soil samples were collected to determine the soil particle composition and soil organic matter contents. It should be noted that the undisturbed soil samples were not replicated due to the possible cost incurred and challenges obtaining the samples. In addition, some soil cores were damaged during drilling. Therefore, the number of soil cores with SHPs that could be measured were 30, 100, and 76 for Yangling, Changwu, and An’sai, respectively. The corresponding soil drilling depths were 104.5, 204.5, and 161.6 m, respectively.

2.3 | Laboratory analysis

$K_s$ was determined for undisturbed soil samples using the constant head method (Wang, Wang, Wei, Shao, & Li, 2008). The soil water retention data were measured by the centrifugation method (Hitachi CR21G centrifuge; 20°C) at suctions of 1, 10, 20, 40, 60, 80, 100, 200, 400, 600, 800, and 1,000 kPa (Lu, Shao, Horton, & Liu, 2004). The BD was determined based on the volume–mass relationship for each oven-dried core sample (105°C, 48 hr; Wang et al., 2008). The disturbed soil samples were also air-dried and passed through a 2.0-mm mesh before measuring the soil particle composition by laser diffraction (Mastersizer 2000, Malvern Instruments, Malvern, UK; Liu, Tong, & Li, 2005). The samples were also passed through a 0.25-mm mesh to determine the soil organic carbon (SOC) contents by dichromate oxidation (Nelson et al., 1982).
2.4 | Data analysis

2.4.1 | SWRC

The SWRC is influenced by many factors, including physical, chemical, and biological processes. Many models have been developed to fit the SWRC, such as the Gardner model (Gardner, Hillel, & Benyamini, 1970), Brooks–Corey model (Brooks & Corey, 1964), Mualem model (Mualem, 1976), van Genuchten (VG) model (Van Genuchten, 1980), and Campbell model (Campbell, 1974). The VG model is commonly used because it can be fitted to SHP data for a wide range of soil textures (Liu, Shu, & Wang, 2007). The equation for the VG model is

\[
\theta(h) = \theta_s + \frac{\theta_r - \theta_s}{1 + (\alpha h)^n} (1 - n h)^{n - 1},
\]

where \(\theta(h)\) is the volumetric water content (cm\(^3\) cm\(^{-3}\)) for the soil water pressure head \(h\) (cm), \(\theta_s\) is the saturated soil water content (cm\(^3\) cm\(^{-3}\)), \(\theta_r\) is the residual soil water content (cm\(^3\) cm\(^{-3}\)), \(\alpha\) is a fitting parameter related to the inverse of the air entry pressure, and \(n\) is a fitting parameter related to the soil pore distribution.

2.4.2 | PTFs

In this study, the 206 soil samples were divided randomly into two groups: Group A (137) for deriving the PTFs (including calibration data sets for SHPs) and Group B (69) for validating the PTFs.

Many methods have been used to develop PTFs, such as multiple linear regression, nonlinear regression, and ANNs. Multiple linear regression is a traditional method for developing PTFs, where it is applicable, and it has been employed in soil science for developing the PTFs for soil parameters (Kai Hua, Shao Hui, Ji Chun, Shu Hua, & Qing, 2011; Li et al., 2007; Santra & Das, 2008; Wang et al., 2012). ANNs have also been applied successfully to the development of PTFs, and these generally perform better than other PTFs (Vereeken et al., 2010; Yao et al., 2015). However, large data sets are needed to obtain good estimates using ANNs (Agvare, Park, & Vlek, 2007; Patil, Rajput, Singh, & Singh, 2009). Therefore, in the present study, stepwise multiple linear regression was performed to select the most significant input variables, before investigating the SWRC soil data (corresponding to the water contents at suction of 1, 10, 20, 40, 60, 80, 100, 200, 400, 600, 800, and 1,000 kPa). The results showed that the coefficients of determination \(R^2\) all exceeded 0.98. Therefore, the soil samples fitted the VG equation well. Table 1 shows the descriptive statistics for the VG parameters and \(K_s\) at all of the sampling sites. The mean values of \(K_s\) and \(\alpha\) ranged from 0.002 to 0.007 cm min\(^{-1}\) and from 0.002 to 0.005 cm\(^{-1}\), respectively. The mean values of \(n\) and \(\theta_s\) ranged from 1.192 to 1.283 and from 0.420 to 0.439 cm\(^3\) cm\(^{-3}\), respectively. The SHPs differed significantly among the sampling sites \((P < 0.01)\). The CV is an indicator of the overall variation of a given variable. At all of the sampling sites, there was high variation in \(K_s\) (CV \(>100\%\), moderate variation in \(\alpha\) (10\% < CV < 10\%), and low variation in \(n\) (except at An'sai) and \(\theta_s\) (CV \(<10\%\); Table 1: Nielsen & Bouna, 1985). Thus, the variations in SWRC in the deep soil profile were small compared with those in \(K_s\) on the Loess Plateau.

In addition, the performance of the new PTFs was determined based on three indexes, the coefficient of determination \(R^2\), the root mean squared error (RMSE), and the mean error (ME), defined as follows:

\[
R^2 = 1 - \frac{\sum_{i=1}^{N}(y_i - \hat{y}_i)^2}{\sum_{i=1}^{N}(y_i - \bar{y})^2},
\]

\[
RMSE = \sqrt{\frac{\sum_{i=1}^{N}(y_i - \hat{y}_i)^2}{N}},
\]

\[
ME = \frac{\sum_{i=1}^{N}(y_i - \hat{y}_i)}{N},
\]

where \(y_i\) is the measured value, \(\hat{y}_i\) is the predicted value, \(\bar{y}\) is the mean of the measured value, and \(N\) is the number in Group A.

2.5 | Statistical analysis

The data were analysed with different software packages. Descriptive statistical analyses (including a calculation of the maximum, minimum, average, and coefficient of variation [CV], Pearson’s correlation analysis, and linear regression analysis were performed with SPSS (version 16.0). Nonlinear regression analysis was conducted for the SWRCs using RETC software (version 6.0).

3 | RESULTS

3.1 | Statistical characteristics of SHPs

We used the VG equation to fit the SWRC soil data (corresponding to the water contents at suction of 1, 10, 20, 40, 60, 80, 100, 200, 400, 600, 800, and 1,000 kPa). The results showed that the coefficients of determination \(R^2\) all exceeded 0.98. Therefore, the soil samples fitted the VG equation well. Table 1 shows the descriptive statistics for the VG parameters and \(K_s\) at all of the sampling sites. The mean values of \(K_s\) and \(\alpha\) ranged from 0.002 to 0.007 cm min\(^{-1}\) and from 0.002 to 0.005 cm\(^{-1}\), respectively. The mean values of \(n\) and \(\theta_s\) ranged from 1.192 to 1.283 and from 0.420 to 0.439 cm\(^3\) cm\(^{-3}\), respectively. The SHPs differed significantly among the sampling sites \((P < 0.01)\). The CV is an indicator of the overall variation of a given variable. At all of the sampling sites, there was high variation in \(K_s\) (CV \(>100\%\)), moderate variation in \(\alpha\) (10\% < CV < 10\%), and low variation in \(n\) (except at An’sai) and \(\theta_s\) (CV <10\%; Table 1: Nielsen & Bouna, 1985). Thus, the variations in SWRC in the deep soil profile were small compared with those in \(K_s\) on the Loess Plateau.

3.2 | Correlation analysis

Before developing the new PTFs, we investigated the possible relationship between the SHPs and soil properties. Table 3 shows the Pearson’s correlation coefficients that were calculated among the variables based on the calibration data sets (Table 2). The results show that there were significant and positive correlations among the SHPs \((P < 0.01)\). For example, \(K_s\) had significant positive correlations with \(\alpha\),
significant correlations between cant correlations with all of the selected variables (Note analysis were used to develop the new PTFs for SHPs (Table 3).

The results obtained by correlation were also high correlations with BD and clay (Note was not an important factor for developed pedotransfer functions)

<table>
<thead>
<tr>
<th>TABLE 3</th>
<th>Pearson correlation analysis between soil hydraulic properties and soil properties</th>
</tr>
</thead>
<tbody>
<tr>
<td>Variables</td>
<td>Ks</td>
</tr>
<tr>
<td>Ks</td>
<td>1</td>
</tr>
<tr>
<td>α</td>
<td>0.42**</td>
</tr>
<tr>
<td>n</td>
<td>0.37**</td>
</tr>
<tr>
<td>θs</td>
<td>0.33**</td>
</tr>
<tr>
<td>BD</td>
<td>-0.54**</td>
</tr>
<tr>
<td>Sand</td>
<td>0.33**</td>
</tr>
<tr>
<td>Silt</td>
<td>-0.26**</td>
</tr>
<tr>
<td>Clay</td>
<td>-0.27**</td>
</tr>
<tr>
<td>SOC</td>
<td>0.14</td>
</tr>
</tbody>
</table>

Note. BD: bulk density; SOC: soil organic carbon.
* Correlation significant at P < 0.05 (two-tailed).
**Correlation significant at P < 0.01 (two-tailed).
which explained 47.4% of the total variation. It is interesting that the capacity for predicting $K_s$ was the highest because it is usually considered to have low $R^2$ values with most PTFs (Wang et al., 2012; Wösten et al., 1999). Although the PTFs developed in previous studies were for predicting $K_s$ only in the upper soil layers of different regions, it is possible that $K_s$ is influenced by only a few factors in the deep soil layers (e.g., soil texture, BD, and SOC), whereas it may be influenced by many factors in the upper layer (e.g., soil texture, vegetation coverage, and human activities). Therefore, our PTFs obtained higher $R^2$ values for the predictions of $K_s$.

In addition, the stepwise multiple regression analysis identified factors that had significant correlations with the SHPs. Among all of the SHPs (except for $n$), BD and sand were important input variables for the regression equations. Thus, BD and sand were important factors for predicting the SHPs in the deep profiles. In addition, BD, clay, and SOC were important input variables for predicting $n$.

The accuracy of the new PTFs was evaluated using the calibration data, and Table 2 shows the values obtained in terms of $R^2$, the RMSE, and ME. The values of $R^2$ and RMSE ranged from 0.481 to 0.566 and from 0.002 to 0.126, respectively, thereby indicating that the accuracies of the predictions differed among the new PTFs. The ME values were all greater than zero, thereby indicating that the SHPs were underestimated by the new PTFs. In addition, the performance of developed PTF models was tested by using the validation data sets (Table 6). The values of $R^2$ and RMSE ranged from 0.375 to 0.625 and from 0.002 to 0.144, respectively, which were similar to that attained by the calibration data sets.

### 3.4 Comparison with existing PTFs

We compared the performance of three existing PTFs (Table 5) and the new PTFs based on the validation data, and the evaluation indexes obtained for the PTFs are shown in Table 6. Figure 2 also compares the performance of the new and existing PTFs by predicting all of the SHPs as scatter plots (except for $K_s$). Compared with the other PTFs, the new PTFs had higher $R^2$ values, whereas the values of RMSE and ME were lower, thereby indicating the improved performance of the new PTFs in the study area. Clearly, there were obvious limitations when applying the PTFs developed for other regions, as shown in other studies (Li et al., 2007; Wang et al., 2012).

We also found that the RMSE and ME values obtained by the other PTFs for $K_s$ were greater than 100 and even up to 1,000, possibly because $K_s$ was much lower in the deep soil layer than the upper soil layer, thereby obtaining poor predictions with the three existing PTFs.

In addition, in terms of the capacity to predict the SHPs of new PTFs and existing PTFs (Table 5), the HYPRES PTFs, which were developed for Europe, ranked second best, and the Li PTFs, which were developed for other regions in China, ranked third best. The databases used for developing the PTFs in the aforementioned studies were different. The PTFs developed by Li comprised data for 63 SWRCs and 36 saturated soil hydraulic conductivities, whereas more than 5,000 were used in the HYPRES PTFs. Therefore, the predictive capacity of the HYPRES PTFs was better compared with that of the PTFs developed by Li.

In this study, we obtained important data for SHPs to study the hydraulic processes and hydrologic models in the ECZ. In addition, we developed the first PTFs for soil SHPs in deep soil layers, and they performed better than existing PTFs. These new PTFs could save time, labour, and money and improve the efficiency of research of the ECZ in the study area.

### TABLE 4 Pedotransfer functions developed for soil hydraulic properties

<table>
<thead>
<tr>
<th>Model parameters</th>
<th>Regression equations</th>
<th>Adjusted $R^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$K_s$</td>
<td>$-1.523 + 1.685^{<em>}BD^{-1}$ $+$ 0.0004</em>Sand $- 0.996*lnBD$</td>
<td>0.561</td>
</tr>
<tr>
<td>$\alpha$</td>
<td>0.012 $+$ 0.0002<em>Sand $- 0.007</em>BD$</td>
<td>0.474</td>
</tr>
<tr>
<td>$n$</td>
<td>$5.507 + 6.966^{<em>}Clay^{-1} - 7.727^{</em>}BD^{-2}$ $+$ 0.186<em>SOC $-$ 4.399^{</em>}BD$^{-1}$</td>
<td>0.526</td>
</tr>
<tr>
<td>$\theta_s$</td>
<td>$-0.779 - 0.608^{<em>}BD^{2} + 0.016^{</em>}lnSand$ $+ 1.712<em>BD - 0.000027^{</em>}Sand^{2}$</td>
<td>0.519</td>
</tr>
</tbody>
</table>

### TABLE 5 Established pedotransfer functions (PTFs) used for comparison with new PTFs developed in this study

<table>
<thead>
<tr>
<th>PTFs</th>
<th>Source database</th>
<th>Methodology to develop PTFs</th>
<th>Hydraulic parameter</th>
<th>Input variables</th>
<th>Country</th>
</tr>
</thead>
<tbody>
<tr>
<td>Li et al. (2007)</td>
<td>Fengqiu County (N = 63 and 36)</td>
<td>Multiple linear regression</td>
<td>$K_s$, $\alpha$, $n$, $\theta_s$</td>
<td>BD, SOC, silt, clay, sand</td>
<td>China</td>
</tr>
<tr>
<td>HYPRES (Wösten et al., 1999)</td>
<td>HYPRES database (N = 5,521)</td>
<td>Nonlinear regression</td>
<td>$K_s$, $\alpha$, $n$, $\theta_s$</td>
<td>BD, SOC, silt, clay, horizon</td>
<td>Europe</td>
</tr>
<tr>
<td>Wang et al. (2012)</td>
<td>The Loess Plateau (N = 252)</td>
<td>Multiple linear regression</td>
<td>$K_s$, $\theta_s$, $\theta_s$</td>
<td>BD, SOC, sand, silt, clay, altitude</td>
<td>China</td>
</tr>
</tbody>
</table>

Note. BD: bulk density; SOC: soil organic carbon; FC: field capacity.
The Loess Plateau area of China is predominantly covered by deep loessial deposits (generally 50–200 m), which are subject to intense soil erosion. However, it is difficult to obtain direct measurements of SHPs for the deep soil layer (generally 50–200 m depth) on the Loess Plateau, thereby making it necessary to employ related PTFs. Until now, PTFs were not available for the SHPs of the deep soil layer on the Loess Plateau. Wang et al. (2012) also developed PTFs for the SHPs on the Loess Plateau, China, but they focused mainly on the upper layer (0–5 cm), which is not sufficiently deep for the Loess Plateau. In addition, the SHPs of the deep soil layer differ from those in the upper layer, especially for $K_s$.

Therefore, we developed the first set of PTFs for the SHPs of the deep layers on the Loess Plateau, China, thereby improving the efficiency of research into the water cycle (such as water movement in the thick unsaturated zone and the pattern of precipitation supplying groundwater) and facilitating the development of relevant hydrological models of the Loess Plateau. This study may contain the first set of PTFs developed for very deep soil layers anywhere in the world, and they may be applicable to deep soil layers in other regions. A limitation of our study was that the number of soil samples was small, which was due to the difficulty of obtaining samples from such deep soil layers. Further research is necessary to obtain more undisturbed soil samples from deep soil layers.

### Conclusion

In this study, we measured SHPs and basic soil properties at three typical sites (Yangling, Changwu, and An’sai) on the Loess Plateau, China. Samples were collected from the top of the soil profile to the bedrock by soil core drilling. We used the results to develop new PTFs by stepwise multiple linear regression. The results showed that at all of the sampling sites, there was high variation in $K_s$, moderate variation in $\alpha$ and $n$ (except at An’sai), and low variation in $\theta_s$. The adjusted $R^2$ values obtained for the new PTFs for SHPs ranged from 47.4% to 56.1%. The PTFs performed best for $K_s$ ($R_{adj}^2 = 0.561$) and worst for $\alpha$ ($R_{adj}^2 = 0.474$). BD and sand were the most important input variables for predicting $K_s$, $\alpha$, and $\theta_s$, whereas BD, clay, and SOC were the most important for $n$. The PTFs developed in this study performed better when compared with existing PTFs. In this study, we obtained important data for SHPs to facilitate the study of hydraulic processes, and we developed the first PTFs for SHPs in deep soil profiles in the ECZ.

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### References


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