Modeling Moisture Retention in Peat Soils

R. Weiss, J. Alm,* R. Laiho, and J. Laine

ABSTRACT

Soil moisture governs many biogeochemical processes in peatlands. Modeling of those processes relative to climate and anthropogenic influences requires knowledge of the basic hydraulic properties of different peat soils in a function form. Water retention of undisturbed soil samples of peat soils collected at four depths at each of 36 undrained and drained pine (Pinus sylvestris L.) mire sites, was measured for suction pressures of $-0.98$, $-3.10$, $-6.19$, $-9.81$, $-98.1$, and $-1554.25$ kPa. The obtained data were used to test several well-known water retention models commonly applied to mineral soils. The most suitable model was found to be van Genuchten’s model if the residual water content was omitted. Peat characteristics were used to explain the variation in the model’s shape parameters. Accounting for the remains of Sphagnum, Carex, Eriophorum, and lignin and the distinction between shallow and deep peat layers considerably improved the moisture retention predictions compared with using bulk density only. The different behavior of the shallow vs. the deep peat layers was mainly attributed to the Sphagnum and lignin residues, but not to the Carex residues. We developed a semiempirical model with only one shape parameter, which was clearly better explained by the peat characteristics than the two shape parameters of the van Genuchten model. We recommend that for statistical investigations or investigations requiring a robust model, the semiempirical model be used. The van Genuchten model is to be preferred in predicting the moisture conditions near saturation.

Peat soil, as a matrix for hydrophysical phenomena, is characterized by a high proportion of small pores (e.g., Päivänen, 1973) and a very heterogeneous pore structure derived from plant residues in various stages of decomposition. According to Loxham (1980), different pore categories can be identified: large multiple and simply connected open pores, dead-end pores, completely isolated pores, and pores in cell structures. The structure of the peat matrix thus elicits a hydrophysical response different from that of the granular geological porous media (Hoag and Price, 1985).

Knowledge of the water content profile of peat relative to the level of the water table is a prerequisite for modeling processes related to soil moisture conditions of peatlands. Most models of water content in porous media make intensive use of a moisture retention curve, which describes the moisture conditions at different pressure heads. The relationship between soil permeability or hydraulic conductivity and soil water content is also in a key position in considering water movement, and is often directly related to the moisture retention curve. Both physical characteristics, however, are seldom available, especially in the case of peat soils and when operating on a regional scale. Fortunately, basic peat soil characteristics are often available for peatland research sites, or are monitored during soil survey campaigns. Equations describing relationships between peat soil characteristics and hydraulic properties could improve the use and interpretation of peat soil maps and increase the applicability of simulation models at both the local and regional scale.

For peat soils, very few attempts have been made to estimate water retention from certain peat properties. Boelter (1969) and Päivänen (1973) used multiple regressions to relate the water content at certain pressure head values to the bulk density of peat. The disadvantage of these models is that they provide data in tabular form, which makes mathematical and statistical operations difficult. A continuous function to better describe the water retention characteristics is preferred. This would enable the generation of complete curves and facilitate both mathematical and statistical operations. Romanov (1968), who dealt with the physical interpretation of pore geometry and capillary rise of water in peat, pointed out that the water retention of peat at static equilibrium could be hyperbolically related to the height of the water table and therefore to the matrix suction. Although hyperbolic curves have, to a limited extent, been published for peat samples by Romanov (1968) and Vorobev (cited by Ivanov, 1981), they were not related to other peat properties.

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The water retention characteristics of mineral soils have been modeled quite intensively, and several models have been presented in the last 25 yr (e.g., Brooks and Corey, 1964; Brutsaert, 1966; van Genuchten, 1980; Ross and Smettem, 1993; Zhang and van Genuchten, 1994). Some of these models could also be calibrated for peat soils, and some will be investigated here. Most of the water retention models for mineral soils allow for analytical solutions of the hydraulic conductivity or permeability function. Unfortunately, these analytical models contain curve shape parameters that were originally determined for large sets of mineral soil samples (e.g., Mualem, 1976). Consequently, they should not be used for peat soils without refitting the shape parameters (Loxham and Burghardt, 1986).

MATERIALS AND METHODS

Undisturbed volumetric peat samples were collected at 38 peatland sites, both undrained and drained, which belong to the peatland which were collected at 38 peatland sites, both undrained and drained, which belong to the following peatland type(s) in the Finnish classification system (Cajander, 1913; see Laine et al., 1986, for current terminology): (i) herb-rich sedge birch–pine fen, (ii) tall-sedge pine fen, (iii) cottongrass–sedge pine fen, (iv) low-sedge Sphagnum papillosum pine fen, and (v) cottongrass pine bog. Brief site type descriptions are also given in Laito and Laine (1994), where the selection of the material is described in detail. The oldest drainage areas sampled had been drained 55 yr before. Of the nearly 5.3 million ha of peatland drained for forestry in Finland, about 35% consists of these peatland type(s) (Keltikangas et al., 1986). They form a continuum from mesotrophic to oligotrophic and ultimately ombrotrophic. The surface peat is Carex dominated in the meso- and meso-oligotrophic sites, but the proportion of Sphagnum residues increases along the gradient toward ombrotrophy. The peatlands studied are located in southern Finland in a region from 61°35' to 62°05'N and 23°30' to 24°55'E.

Three series of peat samples (289 or 250 cm³, sample height 69 or 63 mm) were taken from four depths: 0 to 10, 10 to 20, 25 to 35, and 50 to 60 cm. Zero level was taken as the upper level of the rooting zone, which often corresponded to the lower level of the green moss layer. The samples were deep frozen and stored until further treatment, a standard preservation technique, which is assumed to cause only minimal alterations in the flexible organic matter pore structures.

For the determination of the water retention, about 1.5-cm-thick subsamples were taken from the top and bottom of the samples. This was done to ensure a reasonable measuring time, because the time needed to reach static equilibrium increases more than linearly with increasing sample thickness, especially in organic soil with pore-size distribution dominated by small-diameter, and partly "dead-end", pores.

The water content of the subsamples was determined gravimetrically at suction levels 0.98, 3.10, 6.19, 9.81, 98.1, and 1554.25 kPa (corresponding to pF values 1.0, 1.5, 1.8, 2.0, 3.0, and 4.2, and pressure heads of 10, 30, 60, 100, 1000, and 15,850 cm H₂O, respectively) obtained using pressure plate extractors (Catalog no. 1500 and 1600, Soil Moisture Equipment Corp., Santa Barbara, CA). The pressure applied was ensured by including a hydrostatic pressure buffering system. The water content of each sample was calculated as the mean of the top and bottom subsample values. After extraction at all pressures, the subsamples were dried at 105°C (standard temperature for organic soils) to constant mass. Their dry masses were then added to the dry masses of the sample's remnants determined earlier, and the bulk densities of the whole sample were used to transform the gravimetric water contents to volumetric ones. The botanical composition of each sample was determined microscopically after a short digestion in a 10% KOH solution and staining with safranine (e.g., Heikurainen and Huikari, 1952). One hundred points were counted on each slide, and the object closest to the center of each point was classified into one of the following classes: Carex, Sphagnum, Ericophorum, lignin (including both tree and shrub remains), uncontrollable plant residues, and amorphous mass (see Table 1).

Model Identification and Parameter Estimation

Basic Models

Three basic equations for describing the water retention curves were tested:

1. The equation proposed by van Genuchten (1980):

   \[ \theta = \theta_s + (\theta_r - \theta_s)[1 + (ah)^{\kappa}]^{n-1} \]  

2. The bimodal equation proposed by Zhang and van Genuchten (1994):

   \[ \theta = \theta_s + (\theta_r - \theta_s)[1 + c_1(ah)]/[1 + (ah) + c_2(ah)^{\alpha}] \]  

3. A semi-empirical equation derived in this study (Appendix 1):

   \[ \theta = \exp\left[\ln(\theta_s) - \ln(\theta_r) - \ln(\theta_{ws})\right] \left[\log_{10}(h) + 4.2\right] \]  

where \( \theta \) is the water content (m³/m³) of peat, \( \theta_s \) is the residual water content (m³/m³), \( \theta_{ws} \) is the wilting-point water content (m³/m³ at 1554 MPa), \( h \) is the pressure head in cm H₂O (15 850 cm H₂O, \( \log_{10}(h) = 4.2 \) at the wilting point), \( \theta_r \) is the saturated water content (m³/m³); \( \alpha, m, n \) are parameters defining the van Genuchten curve shape; \( \alpha, c_1, c_2 \) are parameters defining the Zhang and van Genuchten curve shape; and \( k \) is a single parameter defining the semiempirical curve.

The model parameters were obtained as follows:

Water Content at Saturation. A sensitivity study by Vergeet et al. (1989) showed that models like those above are most sensitive to errors in \( \theta_r \). The value of \( \theta_r \) for the models was therefore not obtained from parameter-fitting values when fitting the models to the data, but from the total porosity of peat as a fixed value for \( \theta_r \). This value can be obtained physically from the bulk density of the peat sample, \( \rho \), and the density of solids or specific gravity, \( g \) (e.g., Päivänen, 1973):

   \[ \theta_r = (g - \rho)/g \]  

The values of density of solids in Finnish peats (here \( g \)) have been reported to vary between 1.4 and 1.6 g cm⁻³ (e.g., Puustjärvi, 1970). In this connection, \( g \) was fixed as an average value of 1.5 g cm⁻³. Gas content of saturated peat, which ranges from 0 to 10% (Päivänen and Laine, 1982), was also ignored in our approach.

Water Content at Permanent Wilting Point. The volumetric water content at wilting point \( h = 15,850 \) cm H₂O, \( \theta_{ws} \) was estimated separately for that pressure head by linear regressions of the measurements. Using only bulk density polyominoes (\( p, p' \)) as parameters, we obtained Eq. [5]. Adding botanical residues to the regression parameters somewhat improved the regression performance, and we obtained Eq. [6]. The notation S, L, C, and Er denote here the Sphagnum, lignin, Carex, and Ericophorum content as percentages:

   \[ \theta_{ws}(p) = 4.3 + 67p \]

   \[ R^2 = 0.28 \]
Table 1. Value range and sample distributions of the 152 peat cores analyzed.

<table>
<thead>
<tr>
<th>Bulk density (g cm⁻³)</th>
<th>Sphagnum (S)</th>
<th>Carex (C)</th>
<th>Lignin (L)</th>
<th>Eriophorum (Er)</th>
<th>Amorphous mass (Amor)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean</td>
<td>0.102</td>
<td>24</td>
<td>20</td>
<td>14</td>
<td>11</td>
</tr>
<tr>
<td>SD</td>
<td>0.03</td>
<td>29</td>
<td>24</td>
<td>10</td>
<td>12</td>
</tr>
<tr>
<td>Max.</td>
<td>0.18</td>
<td>97</td>
<td>89</td>
<td>58</td>
<td>58</td>
</tr>
<tr>
<td>Min.</td>
<td>0.04</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

θ₁₀₀₀(p,S,L,C,Er) = 5.3 + 87p - 0.050C - 0.11L

The coefficients of determination are not high (parameters were significant), but the equations are considered sufficient because of the small water content at the wilting point. Adding depth or interaction parameters presented below did not improve these equations.

Residual Water Content. The residual volumetric water content, θ₁₀₀₀ defined at the permanent wilting point of the plants. The parameter θ₁₀₀₀ was used in Models 1 and 2, but was not obtained from the measurements. Mualem (1976) suggested an extrapolation procedure to obtain θ₁₀₀₀ from other matric suction measurement points. However, this extrapolation procedure estimated θ₁₀₀₀ ≈ 0 for 82% of all peat samples in this work. Therefore, θ₁₀₀₀ was estimated by the model-fitting procedures.

Curve Shape Parameters. The values of curve shape parameters of Models 1 to 3 were estimated by applying the Levenberg-Marquardt algorithm (Marquardt 1963; SPSS, Inc., 1988; Press et al., 1992). The estimates of the parameters are further explained using peat characteristics.

Model Selection

A model identification test was performed to compare the performance of the equations and to check the need for all parameters in the equations. In this test, full and reduced versions of Eq. [1] to [3] were samplewise fitted to the observed water retention data of a subset of 25 peat samples with differing peat characteristics or originating from different depths. Very high correlations were found to exist between the curve shape parameters in Eq. [1] and [2]. The full models were thus overdefined for our data set and could be reduced. To obtain a sufficient degree of freedom with respect to our pressure head measurements, the number of fitting parameters had to be restricted to one or two. In the case of Eq. [1], van Genuchten (1980) suggested m = 1 - 1/n, which does not much affect the flexibility in describing the water retention curve. The restriction n ≥ 1 follows from the restriction 0 < m < 1, both due to the fact that diffusion is ≥0 at saturation (van Genuchten and Nielsen, 1985). Setting m = 1 reduces Eq. [1] to a model proposed by Brutsaert (1966) and Endelmann et al. (1974). In the case of Eq. [2], setting c₁ = 1 results in a genuinely s-shaped curve (Zhang and van Genuchten, 1994). When fitting both full and restricted versions of Eq. [1] and [2], the value of θ₁₀₀₀ still became negative for several samples, forcing us to restrict θ₁₀₀₀ to ≥ 0. However, Vereecken et al. (1989) pointed out that θ₁₀₀₀ is the least important parameter in Eq. [1], which allowed us to assume θ₁₀₀₀ = 0 for all samples. Similarly, Eq. [3] was reduced and tested with θ₁₀₀₀ obtained from Eq. [6] and with θ₁₀₀₀ = 0 (Table 2).

We performed an F-test (Pindyck and Rubinfeld, 1991) to check if a reduced model could be used without a significant loss of fit. When comparing the reduced versions of Eq. [1] to [3], we used Akaike's information criteria, the final prediction error criterion (Soderstroem and Stoica, 1989), and the criterion of minimum description length (Rissanen, 1983), see Table 2. According to these criteria, the model reduced from Eq. [1]:

θ = θ₁₀₀₀[1 + (ah)⁻³]⁻¹ + 1

performed best. This model is related to the theories and physical soil properties presented by van Genuchten (1980), but requires two fitting parameters [n, α]. If only one fitting parameter is allowed, Eq. [3] performed best with θ₁₀₀₀ from Eq. [5] or [6] and [6] as the shape parameter.

Sensitivity Analysis and Parameter Distributions

A sensitivity analysis was performed to evaluate the relative importance of the value parameters. The core of the analysis was similar to Vereecken et al. (1989) but we extended the calculations to all pressure heads. Close to saturation, at a pressure head of 10 cm H₂O, both models were most sensitive to changes in θ₁₀₀₀, then to those in n, k, and α (in descending order), whereas θ₁₀₀₀ had only a small effect. The order of importance was gradually reversed with the pressure head increasing to 15850 cm H₂O. Since the groundwater table is very close to the surface in most natural peat soils, we can conclude that n should be more precisely modeled than α or k.

When the models where separately fitted to each of the 152 sample measurement series, the parameter n followed a normal distribution quite well. Parameter α, however, had a skewed distribution, but fortunately log₁₀(α) was closer to normal and was used in the regressions (see below). The shape parameter distribution characteristics and the corresponding responses of the selected van Genuchten model (Eq. [7]) are shown in Fig. 1a and 1b. The figures indicate that the model is sensitive to changes in log₁₀(α) very close to saturation, whereas the slope is greatly affected by n after 10 cm H₂O. For the selected semiempirical model Eq. [3], shape parameter k followed a normal distribution relatively well (Fig. 1c). Figures 1a to 1c show clearly that k combines the patterns of n and α quite well.

RESULTS

Construction of the Final Models

Linear ordinary least square (OLS) regression was applied to explain the variation in the model shape
parameters \( n, \log_{10}(\alpha) \) in Eq. [7]) and \( k \) in Eq. [3]) from the distributions of the peat characteristics (Table 1). The resulting significant peat characteristic variables were then used in the nonlinear regressions, which were used to derive the final models from the entire empirical set. Five different peat character sets were used in the regression analysis (Table 3). The first set consisted only of the polynomial terms of bulk density. Botanical peat components were added to the second set whereas depth by the sampling layer numbers was added to the third set, and both term groups were added to the fourth set. Interaction terms (botanical components with sampling layer) were finally included in the fifth set.

Before running regression analysis, a preliminary data analysis using correlation and principal factor analysis was performed to detect linear relationships between the peat characteristics and to examine the data structure. Most of the botanical components and the bulk density correlated significantly with each other (Table 4). The bulk density \( \rho \) correlated strongly with the botanical components \( Sphagnum \) (S, negative) and amorphous mass (Amor, positive), and quite strongly with lignin (L) and \( Eriophorum \) (Er). The strong negative correlation between \( Sphagnum \) and \( Carex \) (C) could be explained by the observation that peat soils in Finland have mostly S or C as their main component. The positive correlation between the uppermost sample layer (0–10 cm, Layer 1) and S and the negative correlation between Layer 1 and C can be explained by the differences between the respective peat formation processes. \( Carex \) peat consists mainly of root and rhizome residues, a continuous input of which takes place mainly at a depth of 10 to 30 cm. The uppermost 10 cm are typically dominated by \( Sphagnum \) residues also on sites with \( Carex \)-dominated peat lower down. The high positive correlation between Amor and \( \rho \) results from the correlation of humification with these variables. The correlations between the botanical components can also partly be explained by the fact that they are given as percentages. Therefore, an angular transformation \( x' = \arcsin(x) \) was tested (Ranta et al., 1989, p. 46), but was rejected because of poor performance in the final equations. Also the principal factor model had to be rejected, leaving all the peat characteristics in the final models.

A lack-of-fit test, similar to that performed for mineral soil water retention curve parameters by Vereecken et al. (1989), was used to verify the adequacy of the models in Eq. [3] and [7]. Due to deviations from some of the assumptions of this test in our data, the results can only be taken as indicative, and no significance probabilities are displayed in Table 5. To test whether a larger, unrestricted set of independent variables (UR) is significant compared with a restricted set of variables (R) (Table 5), we used the common \( F \) statistic (Pindyck and Rubinfeld, 1991).
The parameters $n$ and $\log_2(\alpha)$ defining the shape of Eq. [7] can be estimated with coefficients of determination of 38 and 61%, respectively. The most important peat soil properties controlling both parameters were the bulk density and the separation between the shallow peat layer (0–10 cm) and the deeper layers.

The parameter $k$ defining the shape model Eq. [3] was estimated with a coefficient of determination of 70%. Bulk density, the $Sphagnum$ content, and the separation between the shallow peat layer and the deeper layers were the most important factors controlling the parameter $k$. The lignin content was not clearly statistically significant when added (sign. $\tau = 0.04$). Adding interaction terms between the sample layer and the botanical components, the $Sphagnum$ and lignin contents clearly showed statistically significant differences in water retention between top layers and deeper layers. This difference was more significant for the $Sphagnum$ content than for the lignin content. However, since the resulting increase in the coefficient of determination was not clearly significant, Set 4 (Table 3) was the most reliable variable set for the shape parameter $k$.

According to the sensitivity analysis, $n$ should be more accurately determined than $k$. This goal was not achieved. The lack-of-fit test also showed that there was not much more to be explained in the variations of $n$, indicating high fitting errors in the distribution of $n$. Consequently, the van Gennuchten model Eq. [7] was too sensitive to be defined by the regressions above, while the semiempirical model Eq. [3] gave a slightly less accurate but more robust estimate of the water content.

The final models were obtained by nonlinear regression, using the Levenberg-Marquardt algorithm (Marquardt, 1963; SPSS, Inc., 1988, p. B35–B47). The linearly obtained parameter values were used as initial values for the iterations. As a final result, the semiempirical model Eq. [3] has its parameter functions for different sets of peat characteristics listed in Table 6. The best van Gennuchten-type model (Eq. [7]) has its parameter functions listed in Table 7. A one-parameter version of Eq. [7] was tested, with $\alpha$ as shape parameter and $n$ fitted to an optimal average value. The resulting model performed quite well ($R^2 = 0.920$) but clearly not as well as the semiempirical model. We must also point out that simple linear regressions reached only $R^2 = 0.809$ for our water retention data.

### Table 5. Shape parameter regression results.

<table>
<thead>
<tr>
<th>Model parameter</th>
<th>Variable set</th>
<th>Significant regression variables†</th>
<th>$R^2$ adjusted</th>
<th>Lack-of-fit test</th>
<th>Significance test, $P(F_{significance})$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$3_b, k$</td>
<td>1</td>
<td>constant, $\rho, \rho^2$</td>
<td>0.473</td>
<td>37.7</td>
<td>1-&gt;2: &lt;0.001</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>constant, $\rho^2, S, C$</td>
<td>0.558</td>
<td>31.0</td>
<td>1-&gt;2A: &lt;0.001</td>
</tr>
<tr>
<td></td>
<td>2A</td>
<td>constant, $\rho^2, Er, L, Amor$</td>
<td>0.545</td>
<td>31.8</td>
<td></td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>constant, $\rho^2, L, Layer 1$</td>
<td>0.602</td>
<td>27.2</td>
<td>1-&gt;3: &lt;0.001</td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>constant, $\rho^2, L, S, Layer 1$</td>
<td>0.696</td>
<td>19.6</td>
<td>2-&gt;4, 3-&gt;4: &lt;0.001</td>
</tr>
<tr>
<td></td>
<td>4L</td>
<td>constant, $\rho^2, S, L, Layer 1$</td>
<td>0.703</td>
<td>19.0</td>
<td>4-&gt;4L: 0.03</td>
</tr>
<tr>
<td></td>
<td>5</td>
<td>constant, $\rho^2, S, C, L, Llay1, Llay1$</td>
<td>0.709</td>
<td>19.4</td>
<td>4-&gt;5, 4L-&gt;5: 0.13</td>
</tr>
<tr>
<td>$1_e, n$</td>
<td>1</td>
<td>constant, $\rho^2$</td>
<td>0.233</td>
<td>2.8</td>
<td>1-&gt;2: &lt;0.001</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>constant, $\rho^2, C$</td>
<td>0.293</td>
<td>2.2</td>
<td>1-&gt;2: &lt;0.001</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>constant, $\rho^2, Layer 1$</td>
<td>0.360</td>
<td>1.2</td>
<td>1-&gt;3: &lt;0.001</td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>constant, $\rho^2, L, Layer 1$</td>
<td>0.377</td>
<td>1.3</td>
<td>2-&gt;4: &lt;0.001; 3-&gt;4: 0.03</td>
</tr>
<tr>
<td></td>
<td>5</td>
<td>same result as for Set 4</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$1_e, \log_2(\alpha)$</td>
<td>1</td>
<td>constant, $\rho^2$</td>
<td>0.295</td>
<td>68.4</td>
<td>1-&gt;2: &lt;0.001</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>constant, $\rho^2, L, C, S$</td>
<td>0.391</td>
<td>58.3</td>
<td>1-&gt;2: &lt;0.001</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>constant, $\rho^2, Layer 1$</td>
<td>0.519</td>
<td>45.1</td>
<td>1-&gt;3: &lt;0.001</td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>$\rho^2, S, C, Layer 1$</td>
<td>0.613</td>
<td>35.2</td>
<td>2-&gt;4, 3-&gt;4: &lt;0.001</td>
</tr>
<tr>
<td></td>
<td>5</td>
<td>same result as for Set 4</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

† $\rho$ = bulk density, $C = Carex$, $Er = Eriophorum$, $L = lignin$, $S = Sphagnum$, $Amor = amorphous mass$, Layer $1 = 0$–10 cm below peat surface, Layer $2 = 10$–20 cm, Layer $3 = 25$–35 cm, Layer $4 = 50$–60 cm.
Table 6. Parameter functions of the semiempirical model (Eq. [3]).

<table>
<thead>
<tr>
<th>Variable set</th>
<th>Parameter</th>
<th>Estimated parameter functions†</th>
<th>$R^2_{%}$ all data</th>
<th>$R^2_{%}$ valid, part 1, 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Set 4</td>
<td>$\theta_0$</td>
<td>$100 - 66.7 \rho$ (peat sample porosity, Eq. [4])</td>
<td>0.940</td>
<td>0.933</td>
</tr>
<tr>
<td></td>
<td>$\theta_{so}$</td>
<td>$5.3 - 87.7 \rho - 0.11 L - 0.05 C$ (Eq. [5])</td>
<td>0.944</td>
<td></td>
</tr>
<tr>
<td></td>
<td>$k$</td>
<td>$0.71(\pm0.10) + 54.0(\pm4.6) \rho^2 + 0.0068(\pm0.0012) C + 0.0088(\pm0.0012) S - 0.38(\pm0.04) L$ Layer 1</td>
<td>0.942</td>
<td>0.932</td>
</tr>
<tr>
<td>Set 5</td>
<td>$\theta_0$, $\theta_{so}$</td>
<td>same as for Set 4</td>
<td>0.942</td>
<td>0.932</td>
</tr>
<tr>
<td></td>
<td>$k$</td>
<td>$0.48(\pm0.14) + 52.5(\pm4.8) \rho^2 + 0.0077(\pm0.0014) C + 0.0111(\pm0.0015) S + 0.0078(\pm0.0031) L - 0.0045(\pm0.0010) L a y 1 - 0.0090(\pm0.0020) L a y 1$</td>
<td>0.944</td>
<td></td>
</tr>
<tr>
<td>Set 3</td>
<td>$\theta_0$</td>
<td>same as for Set 4</td>
<td>0.922</td>
<td>0.911</td>
</tr>
<tr>
<td></td>
<td>$\theta_{so}$</td>
<td>$4.3 - 67 \rho$ (Eq. [5])</td>
<td>0.931</td>
<td></td>
</tr>
<tr>
<td></td>
<td>$k$</td>
<td>$1.33(\pm0.85) + 26.6(\pm3.9) \rho^2 - 0.28(\pm0.05) L a y 1 + 0.21(\pm0.06) L a y 1$</td>
<td>0.919</td>
<td>0.911</td>
</tr>
<tr>
<td>Set 2</td>
<td>$\theta_0$, $\theta_{so}$</td>
<td>same as for Set 4</td>
<td>0.919</td>
<td>0.911</td>
</tr>
<tr>
<td></td>
<td>$k$</td>
<td>$0.61(\pm0.11) + 54.0(\pm5.5) \rho^2 + 0.0076(\pm0.0014) C + 0.0077(\pm0.0014) S$</td>
<td>0.926</td>
<td></td>
</tr>
<tr>
<td>Set 1</td>
<td>$\theta_0$, $\theta_{so}$</td>
<td>same as for Set 3</td>
<td>0.902</td>
<td>0.888</td>
</tr>
<tr>
<td></td>
<td>$k$</td>
<td>$1.91(\pm0.24) - 14.3(\pm5.1) \rho + 104(\pm13) \rho^2$</td>
<td>0.913</td>
<td></td>
</tr>
<tr>
<td>Set 0 2</td>
<td>$\theta_0$</td>
<td>$102.7(\pm8.0)</td>
<td>0.836</td>
<td>0.830</td>
</tr>
<tr>
<td></td>
<td>$\theta_{so}$</td>
<td>$11.4(\pm1.3)$</td>
<td>0.841</td>
<td></td>
</tr>
<tr>
<td></td>
<td>$k$</td>
<td>$1.42(\pm0.15)$</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

† $\rho$ = bulk density, $C = Carex$, $Er = Eriophorum$, $L = lignin$, $S = Sphagnum$, $Amor = amorphous mass$, $Layer 1 = 0-10$ cm below peat surface, $Layer 2 = 10-20$ cm, $Layer 3 = 25-35$ cm, $Layer 4 = 50-60$ cm, $S a y 1 = S \times Layer 1$, $L a y 1 = L \times Layer 1$.

‡ $R^2$ is for the complete model (must not be compared to $R^2$ in Table 5). Set 0 = parameters $\theta_0$, $\theta_{so}$, and $k$ estimated directly from water retention data, not explained by peat characteristics.

§ The right-hand column displays the results ($R^2_{\%}$ valid) of the cross-validation.

The sion model obtained from the first set to the second one and vice versa. The validation test for both sets of soil properties indicated that all the signs of the regression parameters in the models (Eq. [3] with Table 6, Eq. [7] with Table 7) are stable, and that the parameter values did not change significantly. The cross-validated regression models show an $R^2$ for the independent observation sets comparable to both the $R^2$ obtained on the identification data set and the $R^2$ for the complete data set (last columns in Tables 6 and 7). This indicates stable prediction levels, the semiempirical model Eq. [3] yielding slightly more stable predictions than the van Genuchten model Eq. [7].

Cross-validation performed on the peat characteristic parameter selection results from the linear regression procedure (Table 5) indicated that most of the peat property parameters in sets 1 through 5 remain stable and do not show major changes in their degree of significance. The parameters $\rho^2$, $S$, $C$, and $L$ obtained from Set 4 were especially stable. However, the lignin content ($L$) of Sets 4L and 5 was not always significant. Also, in Set 3 of Model [3], the parameter $L$ was 2nd becomes uncertain.

To be able to evaluate the model performance at different pressure heads, coefficients of determination of the model predictions at the local pressure levels are shown in Fig. 2. Regressions through local measurement points depending on the bulk density or its polynomials, i.e., models of the same structure and type as those presented by Boelter (1969) and Pääväänen (1973), are also shown. The results in Fig. 2 clearly show that a major increase in fit has been achieved by the continuous models presented here, especially in the regions close to saturation. For the optimal peat character set (Set 4), the fit of the Models [3] and [7] were only slightly lower than those for the best possible local multiple regressions, but more usable by being continuous. However, the maximum fit limits of the models due to the single sample curve fitting errors show that the predictions could be much better still, especially at lower pressure heads of 0.98 to 6.19 kPa (10-60 cm H$_2$O).

Examples of observed values and estimated water retention curves (Eq. [3], Sets 4 and 5) and (Eq. [7], Set 4) of some Sphagnum, Carex, lignin, and Eriophorum peat samples are given in Fig. 3a through 3h. The examples illustrate the quite good performance of the retention curves, as well as showing the obvious difference in moisture retention between the top layer and the deeper peat layers.

Figures 1b and 3a to 3h illustrate clearly, that Model [7] for some parameter combinations gives a curve that, close to saturation, has exaggerated slope that can cause problems in numerical studies. The problem can be avoided by a simple linear interpolation from the real saturation point to some threshold point at the retention curve (we recommend the curve point at a threshold pressure head of 3-10 cm H$_2$O). In this way, it is also possible to use empirical models for the water content

Table 7. Parameter functions of the optimal van Genuchten model.

<table>
<thead>
<tr>
<th>Variable set</th>
<th>Parameter</th>
<th>Estimated parameter functions†</th>
<th>$R^2_{%}$ all data</th>
<th>$R^2_{%}$ valid.§</th>
</tr>
</thead>
<tbody>
<tr>
<td>Set 4</td>
<td>$n$</td>
<td>$100 - 66.7 \rho$ (peat sample porosity, Eq. [4])</td>
<td>0.944</td>
<td>0.930</td>
</tr>
<tr>
<td></td>
<td>$n$</td>
<td>$1.40(\pm0.05) - 3.56(\pm0.90) \rho + 13.2(\pm4.0) \rho^2 + 0.0007(\pm0.00034) C + 0.0037(\pm0.0018) L a y 1$</td>
<td>0.953</td>
<td></td>
</tr>
<tr>
<td></td>
<td>$n$</td>
<td>$-5.8(\pm3.0) \rho^2 - 0.065(\pm0.0012) C - 0.0018(\pm0.0007) S + 0.53(\pm0.09) L a y 1$</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

† $\rho$ = bulk density, $C = Carex$, $L a y 1 = 0-10$ cm below the peat surface, $S = Sphagnum$.

‡ $R^2$ is for the complete model (must not be compared to $R^2$ in Table 5).

§ The right-hand column ($R^2_{\%}$ valid) displays the results of the cross-validation.
at saturation (e.g., Päivänä, 1973) with Models [3] and [7]. This makes it possible to account for the 0 to 10% gas content in peat at saturation or to use $g_i$ values deviating significantly from the assumed average $g_i = 1.5 \text{ g cm}^{-3}$.

**DISCUSSION AND CONCLUSIONS**

The models developed and tested in this research show that continuous water retention models apply well to peat soils. A reduced version (Eq. [7]) of the van Genuchten model proved to be optimal for the available measurement intensity (number of suction points). Optimal model parameters were the water content at saturation $\theta_s$, determined from sample porosity, and two shape parameters, $n$ and $\alpha$. The residual water content of peat, $\theta_r$, was thus left out of this model.

The $n$ and $\alpha$ shape parameter distributions, which were obtained by fitting the van Genuchten (1980) model Eq. [7] separately to each peat sample water retention measurement series, could be partly explained by bulk density. Addition of the percentage of the botanical components *Sphagnum* and *Carex* increased the determination rate considerably, and these variables proved to be clearly statistically significant. This indicates that the difference in water retention between different peat types can be explained not only by differences in peat characteristics related to bulk density, but also by differences in plant residue cell structure and peat pore geometry (cf., Romanov, 1968).

A distinction between the top sample layer (0–10 cm from the lower level of the green moss layer) and the deeper sample layers (10–60 cm from the reference level) also proved to be a clearly statistically significant variable. The inclusion of this variable considerably increased the determination degree of peat water retention, but could not be further explained by investigating the shape parameters $n$ and $\alpha$ of the reduced van Genuchten model (Eq. [7]). Fortunately, the distribution of the single shape parameter $k$ in the semiempirical model
Eq. [3] could be better explained. The distribution of k revealed that the top vs. deeper layer distinction is mainly due to layer differences in the water retention characteristics of Sphagnum (clearly significant) and lignin (less significant), but not due to layer differences in Carex (clearly not significant) residues. Physically, the layer dependence of the moisture retention of Sphagnum could be explained by differences in pore structure in the shallow vs. deep peat layers. Logically, Sphagnum water retention should be influenced in the same way. The layer dependence of the moisture retention of lignin could be due to a correlation between macropores and lignin content in the top peat layers, or to a lower degree of humification of the lignin residues in the top layers. The different behavior of Carex is in agreement with the reasoning of Romanov (1968), who pointed out that "grass bogs" do not display a predominantly vertically orientated pore structure in the top layers, and thus have markedly smaller layer differences in water movement than Sphagnum bogs.

Because of the higher degree of freedom, Model [7] performs better than Model [3] close to saturation (at a pressure of 0.98 kPa). Where the suction region near saturation (0.5-10 kPa) is of major interest, the best predictions of moisture retention ($R^2 = 0.942$) are given by the final van Genuchten model (Eq. [7], Table 7). In further statistical analyses or general tasks, for instance water retention questions related to ditching, the semi-empirical model (Eq. [3], Table 6) provides a more robust structure with an almost as good overall prediction level ($R^2 = 0.940$). However, this is achieved at the cost of a lower prediction rate in the region around 1 kPa.

Some improvement in the models could perhaps be achieved if the air-entry pressure in situ could be taken into account, which requires denser measurement intensity at low pressure head values (below 3.10 kPa). The sensitivity analyses suggest that some progress in these models could be made by determining thepeat $\theta_o$ more accurately, Päivänen (1973) and Päivänen and Laane (1982) pointed out that the theoretical value of $\theta_o$ obtained from porosity, as in these models, is slightly too large since peat soil even at saturation contains a certain amount of gas, mostly <10% (Päivänen and Laane, 1982). For laboratory samples, porosity (Eq. [4]) still has the advantage of giving a clear, robust estimate for $\theta_o$, and it was therefore kept among the retention curve parameters. Corrections in the water retention curves due to large gas content at saturation or due to deviations of density of solids from the assumed average value can be made afterward by the interpolation correction proposed above, and will thus not affect the water retention curve outside the interpolation interval (0 to 0.5-0.98 kPa).

One should be aware that the models presented here describe the desorption curve (i.e., falling water table). Adsorption (i.e., rising water table) will probably have different moisture retention characteristics. Hysteresis effects (e.g., Poulauvassilis and Childs, 1971; Inlnecki, 1982) were not taken into account. Peat matrix swelling and shrinking are not accounted for either, but could be determined at a more coarse level from bulk density and peat type according to the results by Päivänen (1982). The range of seasonal water table in natural and drained peatlands corresponds to pressure heads from 0 to 100 kPa, thus reducing the potential error in predictions caused by shrinkage.

**ACKNOWLEDGMENTS**

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**APPENDIX**

**Derivation of the Semiempirical Moisture Retention Equation**

In several studies of mineral soil hydrology, the water retention curve is based on the effective saturation of the soil, which is defined as follows:

$$S_{eff} = \frac{\theta_i - \theta_o}{\theta_i - \theta_s}, \quad 0 \leq S_{eff} \leq 1 \quad [A1]$$

Mathematically, this expression is most sensitive to measurement errors at water content near saturation. This is usually not important in upland mineral soils because most calculations deal in this field with the lack of water caused by deep groundwater tables. In peat soil studies, the opposite generally occurs. The water table is often very close to the peat surface, and the water retention near saturation is far more interesting than the water retention near the residual point. We therefore focused on the opposite expression, the effective saturation deficit $D_{eff}$:

$$D_{eff} = \frac{\theta_i - \theta}{\theta_i - \theta_s}, \quad 0 \leq D_{eff} \leq 1 \quad [A2]$$

In field and laboratory measurements of peat, $\theta_i$ is rarely determined. It is more convenient to use $\theta_{sat}$, which necessitates redefining the expression above. Still, we assumed some clear relationship between the redefined effective saturation deficit and corresponding matrix suction values, $\psi$, which gives:

$$D_{eff} = \frac{\theta_i - \theta}{\theta_i - \theta_{sat}} \approx \frac{\psi_i - \psi}{\psi_i - \psi_{sat}} = \frac{\psi}{\psi_i - \psi_{sat}} \quad [A3]$$

We used an empirical approach in this study to obtain this physical relationship. For the whole data set, the mean measured moisture retention values, $\theta_{meas}$, for each pressure measurement point were calculated. A clear nonlinear relationship was found between the effective saturation deficit calculated from $\theta_{meas}$ and their corresponding matrix suction values, $\psi$. To find a mathematical form of this relationship, the water contents $\theta_{meas}$ were changed to their natural logarithms, $ln(\theta_{meas})$, and the matrix suction values to corresponding logarithms, $log_4(\psi)$. Taking one more logarithmic step, we finally got a very strong linear relationship through the origin:

$$ln \left( \frac{ln(\theta_{meas}) - ln(\theta_{meas0})}{ln(\theta_{meas0}) - ln(\theta_{meas,sat})} \right) = k ln \left( \frac{log_4(h)}{4.2} \right) \quad [A4]$$

All data calculated from $\theta_{meas}$ are situated close to this straight line, giving $R_{adj} = 0.996$. Rearranging the expression above in respect to $\theta_{sat}$ and changing $\theta_{meas}$ to $\theta$, we obtained the semi-empirical water retention curve presented here (Eq. [3]). Clearly, the shape parameter $|k|$ is the slope of the line obtained from logarithmic transformations.

**REFERENCES**


