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On the applicability of unimodal and bimodal van Genuchten–Mualem based models to peat and other organic soils under evaporation conditions

Ullrich Dettmann[a,*], Michel Bechtold[a], Enrico Frahm[a,b], Bärbel Tiemeyer[a]

[a] Thünen Institute of Climate-Smart Agriculture, Bundesallee 50, 38116 Braunschweig, Germany
[b] Physikalisch Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig, Germany

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SUMMARY

Soil moisture is one of the key parameters controlling biogeochemical processes in peat and other organic soils. To understand and accurately model soil moisture dynamics and peatland hydrological functioning in general, knowledge about soil hydraulic properties is crucial. As peat differs in several aspects from mineral soils, the applicability of standard hydraulic functions (e.g. van Genuchten–Mualem model) developed for mineral soils to peat soil moisture dynamics might be questionable. In this study, the hydraulic properties of five types of peat and other organic soils from different German peatlands have been investigated by laboratory evaporation experiments. Soil hydraulic parameters of the commonly-applied van Genuchten–Mualem model and the bimodal model by Durner (1994) were inversely estimated using HYDRUS-1D and global optimization. The objective function included measured pressure heads and cumulative evaporation. The performance of eight model set-ups differing in the degree of complexity and the choice of fitting parameters were evaluated. Depending on the model set-up, botanical origin and degree of peat decomposition, the quality of the model results differed strongly. We show that fitted 'tortuosity' parameters τ of the van Genuchten–Mualem model can deviate very much from the default value of 0.5 that is frequently applied to mineral soils. Results indicate a rather small decrease of the hydraulic conductivity with increasing suction compared to mineral soils. Optimizing τ did therefore strongly reduce the model error at dry conditions when high pressure head gradients occurred. As strongly negative pressure heads in the investigated peatlands rarely occur, we also reduced the range of pressure heads in the inversion to a 'wet range' from 0 to -200 cm. For the 'wet range' model performance was highly dependent on the inclusion of macropores. Here, fitting only the macropore fraction of the bimodal model as immediately drainable additional pore space seems to be a practical approach to account for the macropore effect, as the fitting of the full bimodal model led to only marginal further improvement of model performance. This keeps the number of parameters low and thus provides a model that is more easily managed in pedotransfer function development and practical applications like large scale simulations. Our findings point out first options to improve the performance of the frequently-used simple single-domain models when they are applied to organic soils. We suggest further performance evaluation of these models during wetting periods when they are known to fail to describe preferential and non-equilibrium flow phenomena.

1. Introduction

Physical, chemical and biological processes in peatlands are strongly controlled by the specific hydrological conditions of these environments (Dimitrov et al., 2010; Holden et al., 2004; Lafleur et al., 2005), which are in particular the fluctuating high water levels leading to frequently varying conditions in the upper part of the peat. Water levels close to the ground surface throughout the whole year are needed for peat soils to develop from dead plant material under anoxic conditions. Once the hydrological conditions are disturbed, peatland ecosystems react very sensitively, with consequences for the catchment hydrology, peat physical and chemical properties, water chemistry and biodiversity. Land use requiring drainage leads to aerobic conditions in the soil and thus peat degradation (Holden et al., 2004). Generally, natural peatlands

* Corresponding author. Tel.: +49 05315962663.
E-mail address: ullrich.dettmann@ti.bund.de (U. Dettmann).

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store carbon and act as sinks for atmospheric carbon dioxide (Bragazza et al., 2006; Limpens et al., 2008; Minkkinen, 1999). Due to increased microbiological activity, drained peat soils become hotspots of anthropogenic emissions of the greenhouse gases (GHG) CO_2 and N_2O (Maljanen et al., 2010), and the carbon stock decreases. Furthermore, the enhanced mineralization causes the release of nutrients, especially nitrate, and dissolved organic carbon (Holden et al., 2004). Not only Histosols (WRB, 2008), but also other organic soils with a lower soil organic carbon (*SOC*) content meeting the definition of organic soils according to IPCC (2006), are important sources of GHGs (Leiber-Sauheitl et al., 2013). These organic soils have rarely been studied so far. For simplification, we will refer in the following to both peat soils and 'low *SOC*' organic soils as organic soils.

The biogeochemical processes during peat degradation are mainly controlled by the availability of oxygen, which is in turn controlled by the soil moisture (Rodriguez-Iturbe et al., 2001). Hence, the hydrological and biogeochemical processes in a peatland are strongly dependent on the changing hydrodynamic conditions in the unsaturated zone (Kechavarzi et al., 2010). The hydraulic soil properties strongly control the time-variable state variables and fluxes in peatlands like water table depth, evapotranspiration, groundwater recharge, surface runoff and interflow, and thus the whole water balance. As about 95% of the peatlands in Germany are drained for agriculture, forestry or peat mining (Joosten and Couwenberg, 2012), it is important to study the unsaturated flow and transport processes of degraded peats to improve the understanding of the amount and dynamics of GHG emissions and nutrient release. Rewetting helps to mitigate the negative effects caused by the drainage of peatlands. Therefore, numerical simulations of the water flow in the saturated and unsaturated zone are needed to develop optimal rewetting strategies. Commonly, water flow in the unsaturated zone is modeled with Richards' equation. For its application, the hydraulic properties, i.e., the water retention and unsaturated hydraulic conductivity function need to be known.

Hydraulic properties are commonly determined by laboratory measurements on small core samples. Standard methods are the hanging water column and pressure plate apparatus for the water retention curve (WRC) and the constant or falling head experiments for the hydraulic conductivity function ($K(\theta)$). As measuring $K(\theta)$ is difficult, empirical relationships were developed to derive this function from the water retention characteristics and saturated hydraulic conductivity (K_s). Mualem (1976) derived the unsaturated hydraulic conductivity from the pore-size distribution of a soil. Through the interpretation of the WRC as a statistical measure of its equivalent pore size distribution, $K(\theta)$ can be inferred from measured data of the WRC and K_s (van Genuchten, 1980). In his model for $K(\theta)$, Mualem (1976) used the parameters that describe the WRC and two additional parameters K_s and τ. τ is related to the tortuosity structure of the connected pores. Over the last decades, the van Genuchten–Mualem (vGM) model has become one of the most commonly applied models to describe hydraulic properties. However, estimating $K(\theta)$ requires K_s and τ. The parameter τ can only be determined by conductivity measurements at different water contents. Based on data from 45 mineral soils (clays, loams and sands), Mualem (1976) proposed an average value of 0.5 for the pore-connectivity parameter τ. Another issue of the vGM model is that it can only account for a unimodal pore size distribution, neglecting macropores. Based on van Genuchten and Nielsen (1985) and Luckner et al. (1989), Schaap and Leij (2000) pointed out that K_s measurements are sensitive to macropore flow.

Macropore flow is an important process in heterogeneous soils in which larger pores are present. Induced by the larger pores the hydraulic conductivity strongly increases at pressure heads near saturation. When water moves along connected macropore pathways, bypassing the porous soil matrix during wetting conditions, preferential flow and non-equilibrium flow occurs (Šimůnek et al., 2003). Different macropore approaches were developed to improve macropore flow modeling in the unsaturated zone (e.g. dual/multi-porosity models, dual/multi-permeability models) (Jarvis, 2007; Köhne et al., 2009; Šimůnek et al., 2003). Empirical dual/multi-porosity models with effective parameters and assuming a single domain represent the simplest concept. Durner (1994) combined two vGM models weighted by the factor ω to a 'bimodal' model representing the entire pore system. Therefore, the shape of the WRC and unsaturated hydraulic conductivity function, influenced by the macropores, can be depicted more accurately than treating the soil as an unimodal pore system. Although the dual/multi-porosity models can account for the increasing hydraulic conductivity near saturation, they are not able to describe the basic physics of the preferential flow process because Richards equation based single-domain models will produce uniform wetting fronts assuming instantaneous equilibrium (Šimůnek et al., 2003). Nevertheless, Köhne et al. (2009) pointed out, that equilibrium single-domain models often yield results similar to two domain approaches, unless dynamic shrinkage cracks are present. Besides this simple single-domain dual/multi-porosity approach, numerous more complex concepts have been developed over the last decades that are able to describe the non-equilibrium flow process. E.g. Hendriks et al. (1999) introduced a complex macropore geometry model, which is implemented in the SWAP model (Kroes et al., 2008).

The frequently demonstrated importance of accounting for macropore flow is well recognized and hydrological model software for small and large scale applications like, e.g., Hydrus, SWAP, SIMGRO, Feflow, Hydrogeosphere and Parflow provide options to apply both the common unimodal hydraulic functions like the vGM model and bi- or multi-modal approaches (e.g., in Hydrogeosphere, see Brunner and Simmons, 2012). However, our impression is that the unimodal vGM model is still most frequently applied (e.g., Bolger et al., 2011; Ferguson and Maxwell, 2010; Li et al., 2008), e.g., due to computational efficiency reasons or the lack of data on macroporosity. When model calibration worked well in these studies, this showed either that the macroporosity effect was negligible at the specific setting and for the specific objective or that the structural model error could be compensated by other model parameters.

The importance of macroporosity on flow and transport may be even more important for peatland environments (Dimitrov et al., 2010; Holden, 2009). Compared to mineral soils, the hydraulic properties of peat soils differ in several aspects. By definition, they have a high amount of *SOC* (Ad-hoc-AG Boden, 2005). Typically they have high porosities (ε) and distinctive shrinkage and swelling characteristics (Hendriks, 2004). Dependent on the original plant substrate, peat soils are characterized by a high spatial variability of the hydraulic properties (Baden and Eggelsmann, 1963). Within fields and regions the variability can be further enhanced by peat degradation due to drainage causing decreasing ε and *SOC* (Beckwith et al., 2003; Holden and Burt, 2003). For mineral soils, many studies focused on the model performance of the Richards' equation and the influence and sensitivity of certain vGM parameters on model results (Romano and Santini, 1999; Šimůnek et al., 1998). However, studies about organic soils are rare. As organic soils differ in several aspects from mineral soils, the applicability for describing organic soil moisture dynamics with standard flow equations and the influence of different vGM parameters on the model performance should be investigated. Dynamic transient laboratory experiments such as evaporation or multi-step outflow (MSO) experiments are good methods to investigate the accuracy of models. First introduced by Gardner and Miklich (1962), several evaporation methods have been developed (Plagge et al., 1990;

Schindler, 1980; Wendroth et al., 1993; Wind, 1968). With simultaneous measurements of evaporation and pressure heads at different depths, both the WRC and $K(\theta)$ can be directly determined for the same sample. However, this method relies on linearization assumptions about the vertical distributions of water contents and pressure heads, which are only approximately fulfilled. The alternative approach is given by the inverse parameter estimation, in which the parameters of hydraulic functions are optimized by minimizing the deviations between measured and predicted state and flux variables, resulting in optimal parameter sets (Kool et al., 1987). The advantage of the inverse approach is that the most suitable parameter values or ranges are determined simultaneously and thus consistently for both the water retention and hydraulic conductivity function without linearization assumptions. Residuals can be used to quantify model errors.

Very few studies applied inverse parameter optimization to dynamical flow experiments with organic soils. Schwärzel et al. (2006) investigated fen peats in Germany with evaporation experiments and Gnatowski et al. (2009) fen peats from Poland with MSO experiments. Both laboratory experiments were simulated with the Richards' equation and the vGM model. Schwärzel et al. (2006) compared directly derived and inversely optimized hydraulic properties and generally found a good agreement for dry conditions (pressure heads < -100 cm). They explained the deviations between 0 and -100 cm by the very small pressure head gradients at the beginning of the experiment which cause relative high uncertainties in the directly estimated hydraulic conductivity near saturation (see also Šimůnek et al., 1998). Furthermore, they tested the accuracy of the estimated hydraulic functions by forward predictions using data from an additional lysimeter. Hydraulic properties derived from transient field and laboratory experiments described the dynamic of the drying process well. In their MSO experiments, Gnatowski et al. (2009) found a good agreement between measured and simulated outflow. However, the cumulative outflow was the only observation. Hence no predictions about the accuracy of the modeled pressure heads could be made. Neither study has tested the influence of the different vGM parameters and the applicability of the vGM model in detail. Moreover, only a small part of the broad variety of organic soils was analyzed and the studies neglected macropores. As the soil moisture in peatlands is often near saturation, macropore flow is an important pathway in the upper peat layers, causing rapid changes in near-surface water contents with a minor effect on the matrix potential (Dimitrov et al., 2010; Holden, 2009). To our knowledge, no studies tried to describe macropore flow with a bimodal model for organic soils. Dimitrov et al. (2010) modeled the peat subsurface hydrology by coupling the Hagen–Poiseuille equation for gravitational macropore flow and the Richards' equation for matrix flow. They found better water content predictions with this coupled approach as compared to the Richards' equation alone.

In this study, we investigate the applicability of the vGM and the bimodal model to describe the hydraulic gradients and water fluxes for five different organic soils during evaporation experiments. Because our experiments are limited to evaporation conditions, the general problems of single-domain models in modeling preferential macropore flow during infiltration are not investigated in our study. In contrast to previous studies, here we systematically compare the performance of different models (unimodal and bimodal) with different parameter set-ups (fixing or optimizing certain vGM parameters). This is done for a relatively large sample volume compared to common evaporation experiments and thus provides more effective parameters that are needed for large scale hydrologic models. We analyze the impact of fitting K_s and τ which are often fixed to measured or default values. The objective of this systematic analysis is to provide a reference that allows the estimation of model performance that is achieved in practical applications depending on the data availability. Finally, we derive suggestions on which model and parameter configuration to choose when modeling the hydrology of peatlands with vGM and bimodal models.

2. Material and methods

2.1. Site descriptions

Evaporation experiments were performed for organic soils from five different study sites spread over Germany (Table 1). Detailed information about the determination of the parameters in Table 1 is given in Section 2.3. The investigated organic soils cover a broad range of different soil properties with bulk densities (b_d) from 0.06 to 0.60 (g cm^{-3}), porosities (ε) from 63% to 93%, *SOC* from 18% to 46% and saturated hydraulic conductivities (K_s) from 41 to 612 cm d^{-1}.

The Schechenfilz (SF) is one of the last near-natural bog complexes in Germany. Thus, the *Sphagnum* peat from this site is the only pristine and weakly decomposed ($H = 2$ on the von Post scale) soil in the study. The von Post scale of decomposition classifies the degree of peat humification based on the proportion of visible plant remains and soil water color (von Post and Granlund, 1926). As the peat was locked under permanently water saturated conditions, it has the highest *SOC* content of all samples. Due to the high amount of macropores in the *Sphagnum* moss K_s is high (612 cm d^{-1}).

As most peatlands in Germany are drained for agriculture or forestry, all other samples are from sites which are currently drained or had been drained in the past. Typically for organic topsoils in Germany, these peat samples are strongly decomposed ($H = 10$). The two study sites Anklam (AK) and Zarnekow (ZA) are both located in the valley of the river Peene. Both peatlands have riverine fen characteristics and evolved as an association of 'percolation mire', 'terrestrialisation mire' and 'flood mire' (Succow, 2012). The different soil properties result from different land use and drainage histories. AK was rewetted 30 years ago, and the vegetation cover is characterized by a succession to sedges, reeds and willows. Accordingly, the upper part of the soil is interspersed with undecomposed leaves and small branches causing a high K_s value of 610 cm d^{-1} and a high amount of macropores. In contrast, Zarnekow is still drained and used as extensive grassland. The progressive degradation and compaction of the peat can be seen in the K_s value which is an order of magnitude lower than that of AK.

The Spreewald (SW) is an alder forest with an extensive system of drainage channels where organic soils developed from paludification processes (initial accumulation of organic matter over mineral soils) and temporary flooding. The samples were taken in an area where a 30 cm thick organic sediment horizon was formed during a limnic period.

As a result of drainage, peat cutting and deep ploughing, the soil from Großes Moor (GM) is the most degraded peat in this study. After peat cutting, only a shallow (around 30 cm) peat layer had remained and was mixed with the underlying sand. The resulting material shows the highest b_d, the lowest ε and the lowest *SOC* of all investigated soils in this study and thus is most similar to mineral soils.

2.2. Evaporation experiments

For each study site, two replicates of evaporation experiments were conducted with undisturbed samples (diameter: 30 cm, height: 20 cm). For the study site SW, only one replicate could be analyzed due to wrong pressure head readings caused by loose tensiometers.

Table 1
Soil properties (5–25 cm) of the study sites: Bulk density (b_d), porosity (ε), soil organic carbon content (*SOC*) and saturated hydraulic conductivity (K_s).

Site	Location	Peatland type	Peat substrate	Land use/vegetation	Von post	b_d (g cm^{-3})	ε (%)	*SOC* (%)	K_s (cm d^{-1})
Schechenfilz (SF)	47° 48′ N 11° 19′ E	Bog	Sphagnum peat (fibric)	Natural	2	0.06	93	46	612[a] (n = 4) (range: 19–1334)
Anklam (AK)	53° 51′ N 13° 40′ E	Fen	Sedges, reeds, fossil woods (sapric)	Reed, sedges, willows	10	0.16	85	41	610[a] (n = 5) (range: 53–2746)
Zarnekow (ZA)	53° 52′ N 12° 52′ E	Fen	Sedges, reeds (sapric)	Extensive grassland	10	0.36	76	28	41[a] (n = 5) (range: 5–322)
Spreewald (SW)	51° 53′ N 14° 2′ E	Fen	Amorphous organic sediment (sapric)	Alder forest	–	0.35	80	20	–
Großes Moor (GM)	52° 34′ N 10° 39′ E	Bog	Amorphous peat (sapric)	Extensive grassland	10	0.60	63	18	53[a] (n = 6) (range: 7–70)

[a] Median.

The soil cores were taken vertically near the surface by manually hammering PVC rings that were sharpened at the bottom edge into the peat and excavating the whole sample. The samples represented the near-surface layer of the organic soils (5–25 cm). At the grassland and the forest sites, the turf and the litter were removed before sampling. After collection, the samples were sealed with a plastic bag and stored at 4 °C. For the evaporation experiments the samples were sealed at the bottom and placed on a scale (Signum 1, Sartorius, Göttingen, Germany; measuring accuracy 0.1 g). Three tensiometers (T8, UMS GmbH, Munich, Germany; measuring accuracy 5 hPa) with cups of 6 cm length and 2.5 cm diameter were inserted vertically at 5.5 cm, 9.5 cm and 15.5 cm depth. The samples were saturated slowly from the bottom until saturation. After saturation, the evaporation experiments started at pressure head conditions of 0 cm at the top of the sample. The experiments were conducted at room temperature which was given by the conditions in our lab and ranged from 17 to 23 °C for most of the times but sporadically also reached 34 °C due to weak lab ventilation in summer. To speed up the experiments, the soil surface was ventilated by a fan. To avoid measurement errors of the scale, the fan stopped for the weight measurements every 10 min. As organic soils have distinctive shrinkage characteristics, vertical and horizontal subsidence of the sample was measured by placing a grid on the columns. The experiments were terminated when the tensiometer cups of the upper tensiometer reached the air entry value at pressure heads of around −800 cm.

2.3. Basic soil properties

After the end of the experiment, samples were dried at 80 °C for 7 days. Standard mass balance calculations based on the weight at the beginning and end of the experiment, the soil mass and the soil volume yielded b_d and the water content at the beginning and end of the experiment. Here, we assumed the whole porosity to be interconnected and that full saturation was achieved at the beginning of the experiment. The vGM parameter θ_s (see Section 2.5.1) and given ε values in Table 1 thus equal the water content at the beginning of the experiment. In practice, full saturation is difficult to achieve at atmospheric conditions, and entrapped air occurs. Thus real θ_s and ε values are probably higher. *SOC* was measured on a LECO TrueMac CN (LECO Corporation, St. Joseph, Michigan, USA) after sieving and grinding the samples.

For all soils except SW, separate K_s measurements on 250 cm^3 samples were done in the laboratory by constant head experiments. To limit edge effects during sampling, a large block of the fibrous peat from the SF was cut and frozen. After pre-drilling, the steel rings for the constant head experiments were inserted into the frozen peat at a depth of 10 cm. Samples from the other sites were conventionally taken from a small pit in the field.

2.4. Direct determination of soil hydraulic properties

For evaporation experiments, the hydraulic properties can be derived directly or by inverse modeling (Section 2.5) using predefined analytical expressions like the vGM Model (van Genuchten, 1980; Mualem, 1976).

In the direct determination, the WRC and $K(\theta)$ result from the pressure head and total water content data at different time steps by algebraic calculations (Plagge et al., 1990; Wendroth et al., 1993; Wind, 1968). In 1980, Schindler, introduced a simplified evaporation method with tensiometer readings at only two depths. The retention function is derived by the mean water content (θ_i) and the mean pressure heads (h_i) for each time step. As described in detail in Peters and Durner (2008), the water flux through the sample between two time steps (t_{i-1} and t_i) is assumed to be equal to $q_i = z_m \cdot \Delta\theta_i/\Delta t_i$ at the middle of the two tensiometer depths with $\Delta\theta_i$ as mean water content change, Δt_i as time increment and z_m as distance from the bottom of the samples to the middle of the two tensiometer. The hydraulic conductivity (K_i) corresponding to the mean pressure head between two time steps ($\overline{hi}$) is derived by inverting Darcy's law:

$$K_i(\overline{h_i}) = -\frac{q_i}{\Delta h_i/\Delta z + 1} \tag{1}$$

Δh_i is the mean difference between the tensiometer readings and Δz the distance between the upper and lower tensiometer.

At pressure heads close to zero, when the pressure conditions are close to hydrostatic equilibrium conditions, K_i cannot be determined exactly by this method due to the high hydraulic conductivity (Wendroth et al., 1993; Šimůnek et al., 1998). The correct measurement of low gradients is limited by the accuracy of the tensiometers. Furthermore, the direct estimation of the hydraulic properties is based on the assumption that the water contents and pressure heads are decreasing linearly over the sample. This assumption can only be fulfilled approximately and the nonlinearity increases with lower pressure heads in the column (Peters and Durner, 2008).

An advantage of the direct determination of the hydraulic properties is the possibility to account for shrinkage in the derivation of the hydraulic properties by using the decreasing soil volumes from the shrinkage measurements to calculate the volumetric moisture content.

2.5. Inverse determination of soil hydraulic properties

2.5.1. Soil hydraulic functions

Two soil hydraulic functions were used in this paper to describe the soil hydraulic properties by inverse parameter optimization. The first one was the commonly-applied van Genuchten–Mualem function (van Genuchten, 1980; Mualem, 1976):

$$\theta(h) = \theta_r + \frac{(\theta_s - \theta_r)}{\left(1 + (\alpha h)^n\right)^m} \tag{2}$$

$$S_e(h) = \frac{\theta(h) - \theta_r}{\theta_s - \theta_r} = \frac{1}{\left(1 + (\alpha h)^n\right)^m} \tag{3}$$

$$K(\theta) = K_s S_e^{\tau}\left[1 - (1 - S_e^{1/m})^m\right]^2 \tag{4}$$

where h (cm) is pressure head, θ, θ_r and θ_s (cm^3 cm^{-3}) are the current, residual and saturated water contents. α (cm^{-1}), n (–), m (–) are empirical parameters where m is calculated by $m = 1-1/n$. S_e is the effective saturation of the sample.

As a second approach, a bimodal model (Durner, 1994) was used for a more accurate description of the hydraulic properties, especially at high water contents. Following Durner (1994), the porous medium can be divided into i overlapping vGM functions weighted by factor ω_i.

$$S_e = \sum_{i=1}^{k} \omega_i \left(\frac{1}{1 + (\alpha_i h)^{n_i}}\right)^{m_i} \tag{5}$$

with the sum of ω_1 to ω_k being equal to 1. Further analysis is restricted to the bimodal model with $k = 2$. By combining the bimodal retention functions with Mualem's (1976) pore-size distribution model, the bimodal unsaturated hydraulic conductivity can be described with the following equation (Priesack and Durner, 2006).

$$K(S_e) = K_s\left(\sum_{i=1}^{k}\omega_i S_{e_i}\right)^{\tau}\left(\frac{\sum_{i=1}^{k}\omega_i\alpha_i\left[1 - \left(1 - S_{e_i}^{1/m_i}\right)^{m_i}\right]}{\sum_{i=1}^{k}\omega_i\alpha_i}\right)^2 \tag{6}$$

During inverse modeling, the secondary pore system leads to higher fitted saturated hydraulic conductivities. The unimodal vGM function depicts the saturated hydraulic conductivity by fitting the function predominantly to the data of the soil matrix, and thus the shape of the hydraulic properties in the macropore range cannot be described (Durner, 1994).

2.5.2. Modeling scheme

The numerical forward modeling was conducted using the finite-element code HYDRUS-1D (Šimůnek et al., 2013) which numerically solves the Richards' equation (Richards, 1931). According to the location of the tensiometers, observation nodes were placed at 5.5 cm, 9.5 cm and 15.5 cm depth. The soil profile (20 cm) was discretized into 100 elements with an element refinement towards the top. Simulations were started at full saturation ($h = 0$ cm at top). The top boundary condition was set to atmospheric with the evaporative water loss during the experiment (cm h^{-1}) as potential evaporation rate. The bottom boundary was set to no flow. All simulations were terminated when the measured upper tensiometer readings reached the minimum pressure head of −800 cm.

Global inverse parameter optimization was performed with the 'Shuffled complex evolution' (SCE-UA) algorithm of Duan et al. (1992). The differences between measured and simulated pressure heads and evaporation rates were minimized by using an objective function (Φ) defined in Šimůnek et al. (1998):

$$\Phi(\mathbf{b},\mathbf{p}) = \sum_{j=1}^{m} \upsilon_j \sum_{i=1}^{n_j}\left[p_j^*(t_i) - p_j(t_i,\mathbf{b})\right]^2 \tag{7}$$

where m describes the two different sets of measurements, i.e., pressure heads and evaporation rates, n_j is the number of measurements of the jth measurement set, $p_j^*(t_i)$ and $p_j(t_i,b)$ are the observations and predictions at time (t_i) for the jth measurement set, $\mathbf{b}$ is the parameter vector, and υ_j is a weighting factor.

The contributions of the two measurement sets to the objective function were normalized by measured data variances σ_j^2 and n_j:

$$\upsilon_j = \frac{1}{\eta_j \sigma_j^2} \tag{8}$$

2.5.3. Model set-ups and parameter limits

As hydraulic experiments with organic soils are rare, we applied different model set-ups to analyze how the parameters influence the model performance of both the vGM and the bimodal model.

All model set-ups were run for pressure heads at the upper tensiometer from approximately 5.5 cm at the beginning to approximately −800 cm at the end of the experiment. For simplicity this range is referred to as **full range**. According to logged tensiometer readings at the sampled field sites over the last 2 years that showed a value of −150 cm at 10 cm depth as the lowest pressure head, a wet pressure head range has been defined from 5 to −200 cm at the upper tensiometer, and the experimental data from drier conditions were not considered during inverse parameter estimation. This set of model runs focused on the derivation of appropriate hydraulic properties for the wet field conditions and is referred to in the following as **wet range**.

Table 2 gives an overview on the realized model set-ups. All set-ups were performed for the wet and the full pressure head range. θ_s was set to a fixed value for all model set-ups according to the saturated water content at the beginning of the experiment. θ_r, α and

Table 2
Overview of model set-ups (fit: parameter was fitted, measured: parameter was fixed to separately determined value).

Model	θ_r (cm^3 cm^{-3})	α (cm^{-1})	n (–)	K_s (cm d^{-1})	τ (–)	ω (–)	α_2 (cm^{-1})	n_2 (–)
3p	Fit	Fit	Fit	Measured	0.5	–	–	–
4p	Fit	Fit	Fit	Fit	0.5	–	–	–
4p_t	Fit	Fit	Fit	Measured	Fit	–	–	–
5p	Fit	Fit	Fit	Fit	Fit	–	–	–
4p_d	Fit	Fit	Fit	Measured	0.5	Fit	1	10
5p_d	Fit	Fit	Fit	Fit	0.5	Fit	1	10
6p_d	Fit	Fit	Fit	Fit	Fit	Fit	1	10
8p_d	Fit	Fit	Fit	Fit	Fit	Fit	Fit	Fit

Table 3
Overview of parameter limits.

Parameter	θ_r (cm^3 cm^{-3})	α (cm^{-1})	n (–)	K_s (cm d^{-1})	τ (–)	ω (–)	α_2 (cm^{-1})	n_2 (–)
Limit	0–0.5	0.002 – 0.5	1.01 – 2.5	0.12–120000	−10–30	0–0.4	0.02–1	1.5–10

n were optimized in all experiments. Further, we compared the performance of models with K_s fixed to the median of the directly measured values with ones in which K_s is optimized. We stress that the directly measured K_s values were determined at separate smaller samples. They are thus not 'directly' measured in a strict sense, as they were not determined for the large samples. As K_s measurements are generally highly variable, measured values at the small samples showed rather large variation. The applied directly measured K_s values are the medians of the measurements (Table 1). All parameter limits are listed in Table 3.

Durner (1994) pointed out that the failure of conductivity estimation methods can mostly be attributed to incorrect values of τ. Mualem's (1976) proposed value of 0.5 was often applied as default in subsequent studies. As no organic soils were included in his original data set, the applicability to organic soils is questionable. Hence, in this study differences in model accuracy were determined by running models with optimized τ and with τ of 0.5.

For the bimodal model, ω was fitted in all cases. One model set-up included the fitting of all three additional parameters. To lower the model complexity of the bimodal model, also set-ups with fixed α_2 and n_2 values were conducted with $\alpha_2 = 1$ and $n_2 = 10$. These values were set very high to represent only the very large macropores.

3. Results and discussion

3.1. Impact of model set-ups on model performance

All model set-ups from Table 2 were applied to all soils. Fig. 1 shows the objective function value Φ for all model set-ups for the **full** (Fig. 1a) and **wet range** (Fig. 1b). Despite the normalization of Φ with the data variances (Eq. (8)), lower Φ were observed for the wet range. The better fits can be explained by the hydraulic gradients that occurred for the wet range, which are closer to hydrostatic equilibrium than for the full range, a situation that is more easily reproduced by the model as pressure heads at hydrostatic equilibrium can be described by the retention function solely. Hence the fits are less dependent to the fit of the hydraulic conductivity function. Therefore, any structural model errors, arising by the simultaneous description of retention and unsaturated hydraulic conductivity function are less affecting model performance than for the full range where gradients in the columns are higher.

Large variances of Φ for a specific model set-up indicate that the performance of this set-up strongly depends on the soil type. It is apparent that the fitting of some parameters lead to a high improvement of the model performance. This is further analyzed in detail with cross-plots (Figs. 2, 3 and 6) in which one parameter is changed individually from 'fixed' to 'fitted', while keeping the rest of the model set-up the same. With these plots, the influence of single parameter for different soils can be illustrated. In these cases, fitting one additional parameter always leads to an equal or lower Φ due to an additional degree of freedom. However, if the model set-up changes in the sense that the model structure is changing (e.g. a sensitive parameter is fixed and additional parameters are fitted), more parameters do not obligatorily lead to a better model performance (e.g. for the full range 5p_d performs worse than 4p_t, see Fig. 1a). A complete list of all optimized parameters and Φ of all model set-ups is given in an on-line supplementary table.

3.2. Impact of fitting τ

Schwärzel et al. (2006) found only minor improvements when varying τ and consequently used $\tau = 0.5$ as suggested by Mualem (1976). In contrast, in our study we found a high sensitivity of the model performance on τ. The highest sensitivity was observed for the samples with high gradients in the column. High gradients have been observed for SF and SW, less distinctive gradients for ZA and low gradients for AK and GM. Fig. 2 compares Φ of the model set-ups with τ fixed to 0.5 and Φ of the model set-ups in which τ was optimized. Fig. 2 indicates that the fitting of τ strongly reduces Φ value in most cases, especially for the pressure head range from 0 to −800 cm referred to as full range (Fig. 2a).

For the **full range** (Fig. 2a), the most pronounced improvements of Φ can be observed for the *Sphagnum* peat (SF), the amorphous organic sediment (SW) and the degraded peat of Zarnekow (ZA). For the degraded peat of Anklam, $\Delta\Phi$ is almost one order of magnitude smaller. Only low pressure head gradients were measured for the AK samples even at dry conditions, indicating a relatively high hydraulic conductivity even at dry conditions. This turns τ into a weakly sensitive parameter for fitting the experimental data. For the amorphous peat of GM, even at low pressure heads, gradients in the columns were still relatively low. The fitted τ values ranged between 0.25 and 3.06 and are relatively close to the default value for mineral soils (0.5) that was applied to the reference model set-ups. Hence, for GM, τ has a low sensitivity on the model performance, also shown by almost the same Φ comparing the model set-ups.

For the other soils the optimized τ values are negative (−1.5 to −4.4), except for the 4p_t model from AK ($\tau > 2$). Negative τ values lead to a less steep decrease of the unsaturated hydraulic conduc-

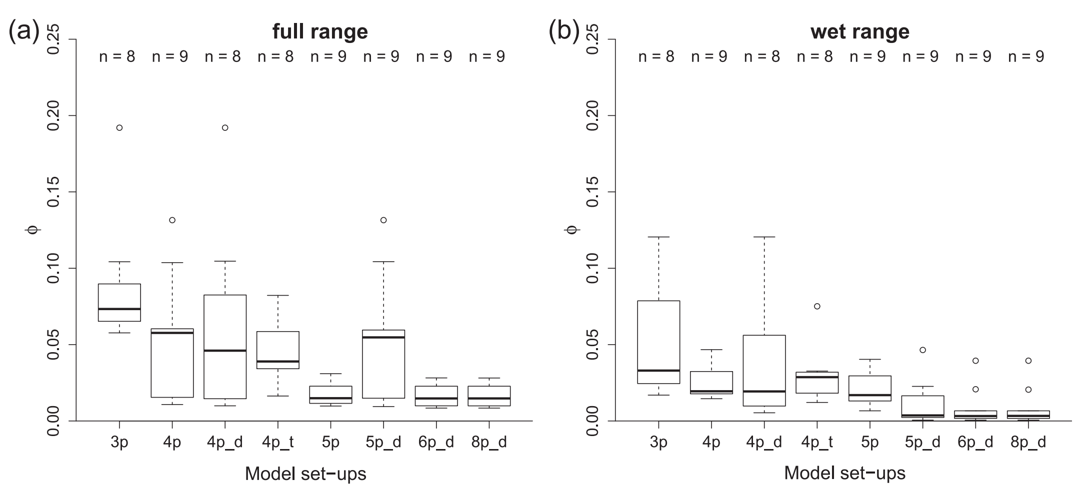

Fig. 1. Objective function value (Φ) of different model set-ups for all sites for full range (a) and wet range (b). For description of the used model set-ups see Table 2.

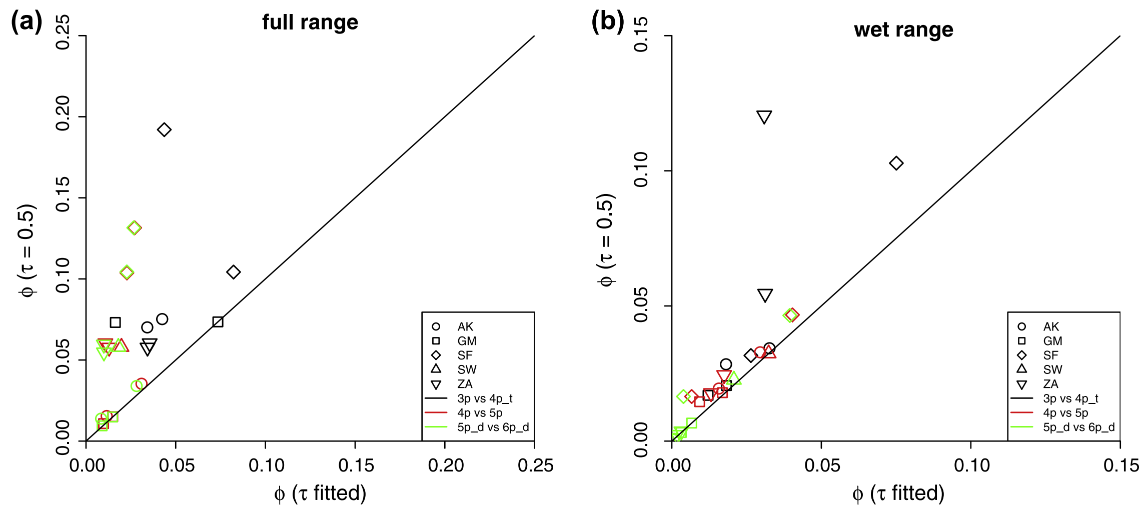

Fig. 2. Sensitivity of model performance on fitting parameter τ. Objective function value (Φ) of model set-ups in which τ was set to 0.5 is plotted vs. the ones in which τ was fitted, while keeping the rest of the model set-up the same.

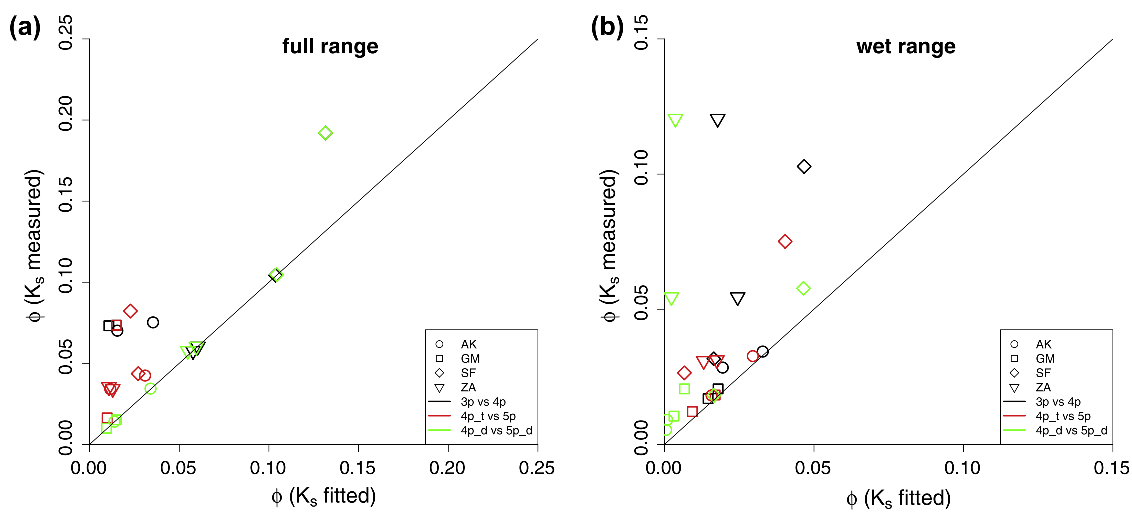

Fig. 3. Sensitivity of model performance on fitting parameter K_s. Objective function value (Φ) of model set-ups in which K_s was fixed to the measured value is plotted vs. the ones in which K_s was fitted, while keeping the rest of the model set-up the same.

tivity function with decreasing pressure heads. Thus, high evaporation rates can be sustained at lower pressure heads. The results coincide with those of several authors which observed a rather small decrease of the hydraulic conductivity function with increasing suction (corresponding to negative τ values) for organic soils. Price and Whittington (2010) fitted simultaneous water retention data and unsaturated hydraulic conductivity data to vGM parameter using the RETC code of van Genuchten et al. (1991). They found negative τ values ranging from -1.81 to -4.38 for a *Sphagnum* peat. A data set of evaporation experiments on organic soils collected by Schindler and Müller (2010) also showed rather small decrease of the hydraulic conductivity with increasing suctions. To our knowledge, this data has not been analyzed further. A more detailed comparison with this data is therefore difficult to conduct. The mostly negative τ values resulting from our optimizations and the studies above indicate a less steep decrease of the unsaturated hydraulic conductivity than would be predicted with the default value of $\tau = 0.5$. There might be two reasons for this. First, the influence of τ on the model performance may be related to the measured shrinkage in the experiments. The samples with the highest shrinkage (SF and SW, shrinkage ~15–20%) showed the strongest improvement of Φ when optimizing τ. For the soils with less shrinkage (e.g. GM, shrinkage ~5%), the reduction of Φ was less distinctive. Rezanezhad et al. (2009) pointed out that the main factors controlling hydraulic conductivity are the tortuosity, porosity and the hydraulic radius of the pores. Bearing in mind that τ is related to the description of the tortuosity with decreasing water contents, our results indicate that τ is able to partly account for the impact of the shrinkage on the unsaturated hydraulic conductivity. Beside the aspect of shrinkage, the very negative τ values that are needed to reproduce the less steep decrease of the unsaturated hydraulic conductivity also may hint to a structural deficit of the vGM model, representing the soil as a capillary bundle, neglecting film and corner flow (Peters, 2013). Accounting for these flow contributions may probably also help to describe the less steep decreasing conductivity function. Gnatowski et al. (2009) found τ values for herbaceous peat (reed and sedge, H_4 to H_7) generally greater than 0 and for moss peat (fibrous structure) samples τ values from -5 to 5. As Gnatowski et al. (2009) performed MSO experiments with cumulative outflow as the only observation in the objective function, the results are not so comparable.

For the **wet range** (Fig. 2b), the improvement gained by fitting τ is much smaller compared to the full range (Fig. 2a), except for the *Sphagnum* peat and the '3p vs. 4p_t' comparisons. Comparing the '3p and 4p_t' model set-ups shows a strong reduction of Φ also for the wet range, except for one sample of GM (Fig. 2a and b) and one sample of AK (Fig. 2b). Parameter τ is a shape parameter in the unsaturated hydraulic conductivity function, and thus it can partly compensate for errors introduced by the fixed measured K_s values in these cases. However, for all other comparisons and soils, even if the range of the optimized τ values is quite large, the default value of $\tau = 0.5$ can be used to model the investigated peat soils for the wet range with an acceptable accuracy. Results indicate that τ is a less sensitive parameter in the wet range.

The analysis of the influence of fitting τ on the model performance showed that when considering the full pressure head range τ represents a crucial parameter for modeling flow in peat soils. Fitted values of τ strongly differed from the default value of 0.5 commonly used for mineral soils. However, from field tensiometer data at the sample sites, we know that these quite low pressure heads do not occur at field conditions in depths of 10 cm or deeper in our investigated soils. They may occur in the upper centimeters (0–10 cm depth) very rarely during the year. Depending on the intended model application and the objective of a peatland hydrological study (e.g., analysis and modeling of peatland water level fluctuations), it might be more important to produce an accurate model for the smaller pressure head range (0 to −200 cm). If lower pressure heads occur during dry periods, the model application should be adapted to these conditions and it is advisable to use the full range models.

The Φ values of the two replicates from the soils mostly show good agreement, except for some 3p and 4p_t set-ups.

3.3. Impact of fitting K_s

The optimization of K_s leads to a strong reduction of Φ. This is shown for almost all model set-ups and soil samples in this study (Fig. 3). For the **full range**, Fig. 3a indicates that in the bimodal model set-ups (green symbols) K_s is not a very sensitive parameter. Although the fitted K_s varied from the measured one (Fig. 4), the fitting only weakly improved the results, except for the *Sphagnum* peat. Conversely for the **wet range**, K_s shows to be a sensitive parameter for the bimodal model set-ups, too.

As described in the Sections 1 and 2.5.3, fitting of K_s leads mostly to K_s values that are lower than ones measured directly at full saturation. As seen in Fig. 4 this effect is not valid for all samples.

For the **full range** (Fig. 4a), the K_s values generally increase from unimodal to bimodal models, except for the *Sphagnum* peat for which no general trend can be observed. For the unimodal models all fitted K_s values were lower than the measured except for the 4p model set-ups from the *Sphagnum* peat and the 4p model set-ups from ZA. This agrees with common results on mineral soils (Schaap and Leij, 2000; van Genuchten and Nielsen, 1985). Generally, the K_s values from the bimodal models were higher than the measured ones. For some cases, e.g., ZA (4p, 6p_d, 8p_d) and SF (4p), the fitted K_s values have a good agreement to the measured ones.

For the **wet range** (Fig. 4b) the fitted K_s values are higher than those of the full range. As for the full range, the *Sphagnum* peat shows a different characteristic with no general trend with higher measured K_s values than fitted. For the other soils almost all fitted K_s values were higher than the measured ones except for one set-up of GM (4p) and the two 4p set-ups of AK. In contrast to the full range, no general trend between unimodal and bimodal models could be observed for the wet range.

3.4. Importance of macropores

Dimitrov et al. (2010) demonstrated the importance of macropores for the modeling of the hydrology of peatlands. In the evaporation experiments of our study, the influence of the macropores can be seen at the beginning of the experiments at pressure heads from 0 to −60 cm. The low water holding capacity of the macropores and the high amount of water stored in the macropores lead to slowly decreasing pressure heads despite high evaporation rates, as shown as an example for one in Fig. 5.

As the unimodal vGM model cannot account for the macropores of a bimodal pore size distribution, the high evaporation rates and quickly decreasing water contents at the beginning of the experiment lead to lower simulated pressure heads than measured pressure heads (Fig. 5a). A solution is given by the simulated bimodal model set-ups, shown, for example, in Fig. 5b. Notice the good agreement between simulated and measured pressure heads between 0 and −60 cm.

The strong improvement of the model performance seen in Fig. 5b is also demonstrated in Fig. 6 by comparing Φ of the unimodal and bimodal model set-ups. Accounting for macropores leads to lower Φ, in particular for the wet range (Fig. 6b).

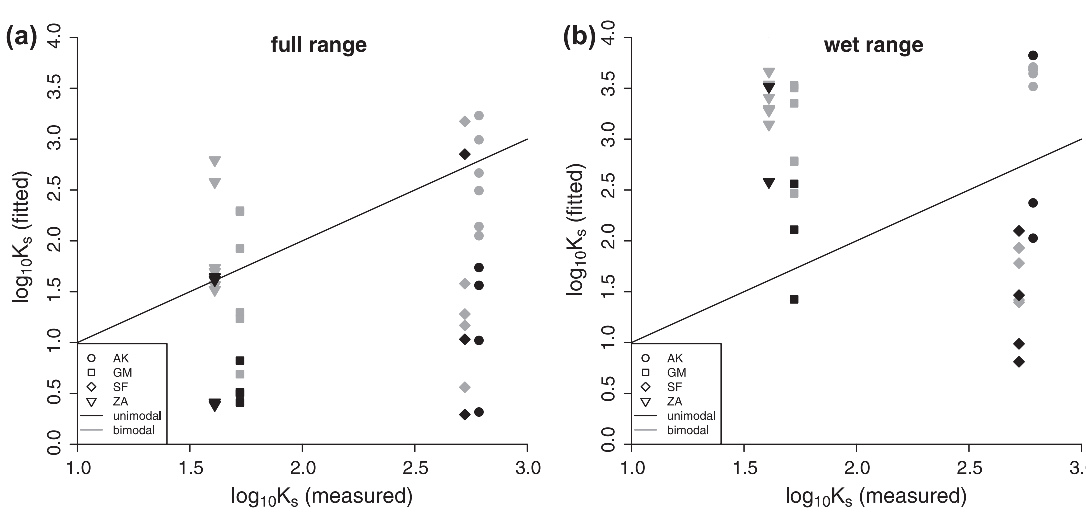

Fig. 4. K_s fitted vs. K_s measured, without the model set-ups were K_s was set to the measured values (3p, 4p_t, 4p_d).

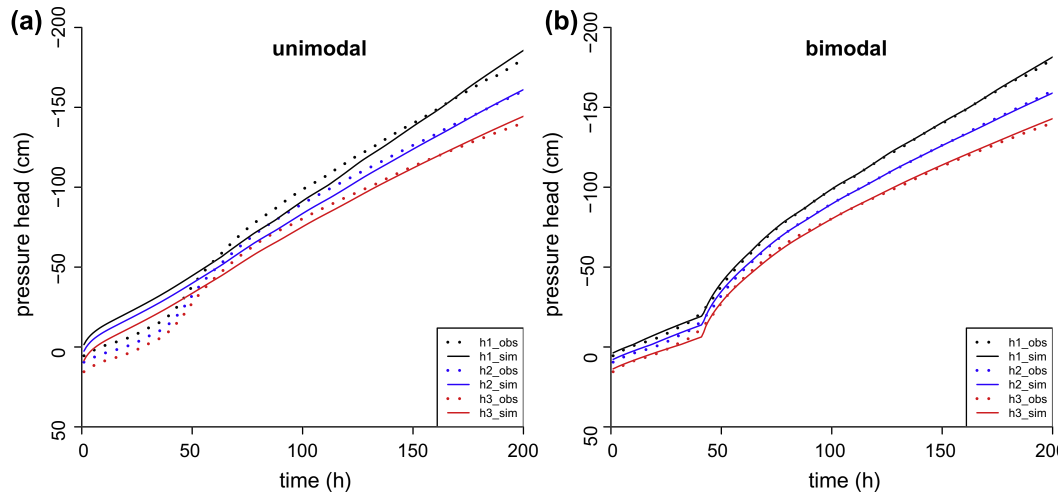

Fig. 5. Measured and simulated pressure heads for AK1 for wet range. (a) unimodal 5p model, (b) bimodal 6p_d model. Legend: Measured pressure heads '_obs', simulated pressure heads '_sim' for the upper 'h1' (−5.5 cm), middle 'h2' (−9.5 cm) and bottom 'h3' (−15.5 cm) tensiometer.

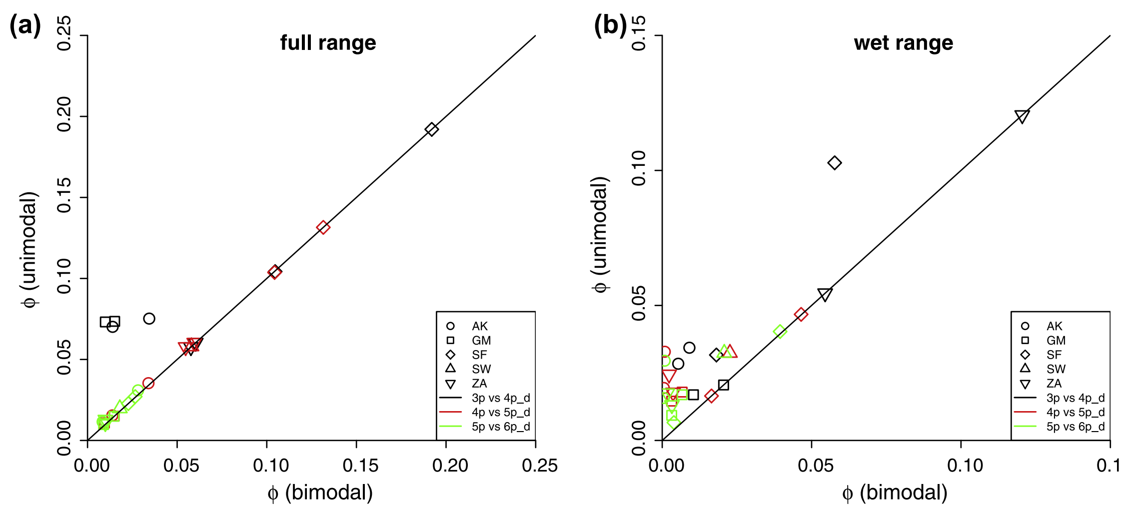

Fig. 6. Objective function value (Φ) of unimodal vs. bimodal model set-ups.

For the **full range** (Fig. 6a), the bimodal model set-ups only improve the model performance for the '3p vs. 4p_d' set-ups. As the 3p set-ups are generally the worst simulations (Fig. 1), the flexibility increases with one additional parameter given in the 4p_d set-ups. For the other bimodal set-ups, Φ is generally dominated by the fit in the dry range with less weight on the pressure head range of the macropores. Hence, the improvement of the model performance appears to be comparatively low.

For the **wet range** (Fig. 6b), almost all samples show a strong reduction of Φ from a uni- to a bimodal model set-up. For samples from AK, the bimodal model leads to the strongest relative improvement. The peat soil of this site, which is covered by willows, contains leaves and branches in the upper part of the soil. The high fraction of larger spaces between the plant residues causes the most pronounced macropore effect for the AK samples. Results for ZA also show the importance of using a bimodal model, which, however, cannot be explained by large spaces between coarse plant residues, as this site is used as extensive grassland. Instead, the sapric horizon is characterized by aggregates which characteristically develop in degraded peat soils. A bimodal pore size distribution seems to be given by the inter-aggregated pores. In the case of the *Sphagnum* peat, the bimodal models do not improve model performance for the '4p vs. 5p_d' and the '5p vs. 6p_d' comparisons. An indication for a bimodal pore size distribution of the *Sphagnum* peat can be seen in Fig. 7c for the directly derived water retention function at only about −400 cm. As the model set-ups for the wet range terminate at −200 cm, the unimodal vGM model was able to depict the hydraulic properties well without a bimodal model. Starting from already good performances, the Φ for the amorphous organic soils (SW, GM) are further improved by the bimodal models.

For all cases, no stronger differences in Φ between the '6p_d and 8p_d' model set-ups have been found (Fig. 1). The optimized values of α_2 and n_2 for the wet range often reached values close to the upper parameter limit of $\alpha_2 = 1$ and $n_2 = 10$. These parameter limits are already very high and a further increase would not lead to much better model performance but rather to an increased instability of the numerical solution. The results indicate that the simplified bimodal model, that uses fixed values for $\alpha_2 = 1$ and $n_2 = 10$ and thus only accounts for the fraction of the largest macropores, is a practical approach to obtain accurate model results.

3.5. Peat soil hydraulic properties and suggestions for practical applications

In Fig. 7a a set of selected model set-ups is compared with directly derived hydraulic properties for one sample of the study sites AK referred as AK1 (Fig. 7a and b) and SF (referred as SF2)

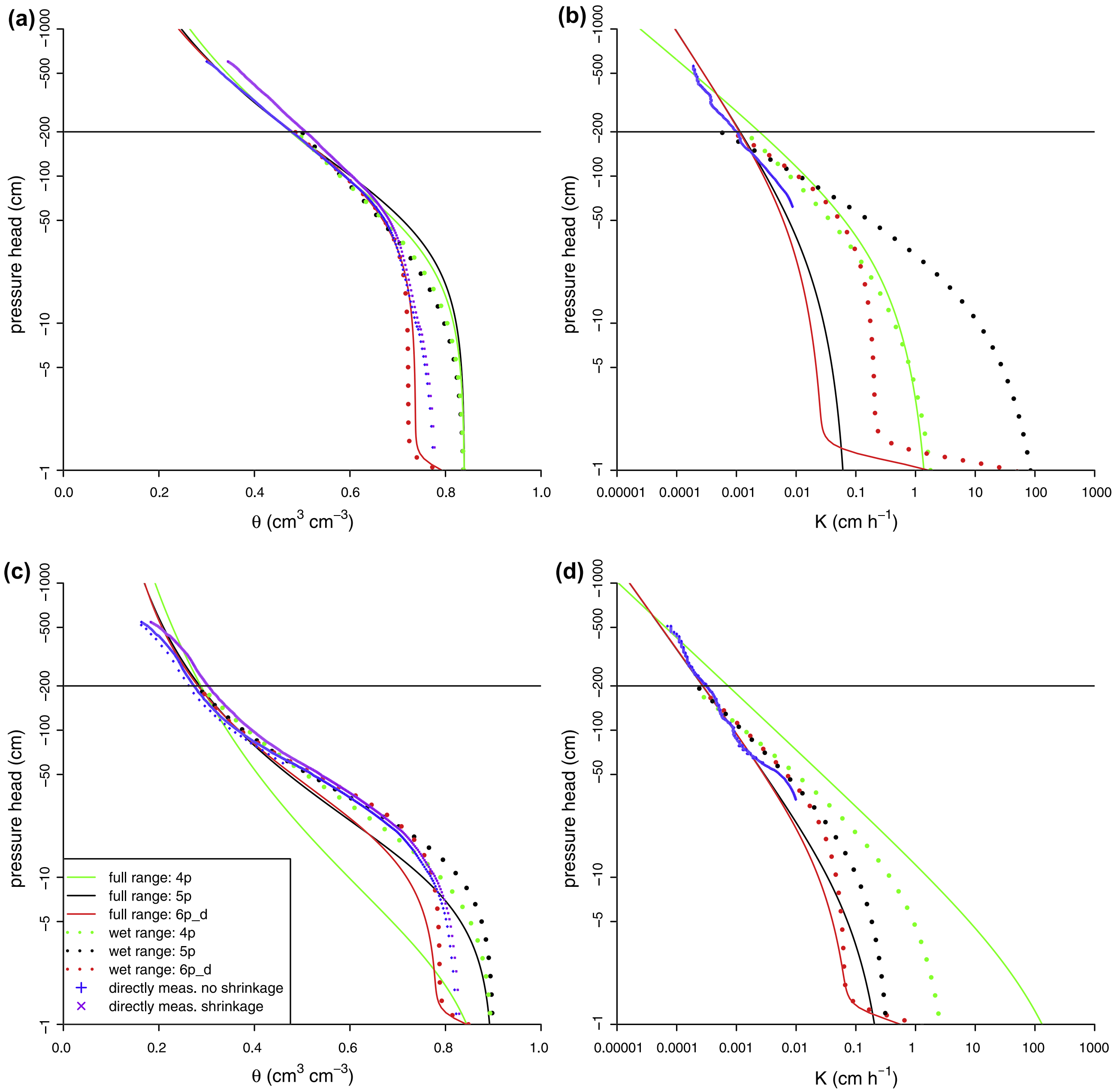

Fig. 7. Directly- and inversely-derived water retention curve for AK1 (a) and SF2 (c) and unsaturated hydraulic conductivity for AK1 (b) and SF2 (d).

(Fig. 7c and d). It is noticeable that the difference between the two retention curves that are based on two different water contents, one of them accounting for the volume loss due to shrinkage, the other not, is rather small compared to the differences between functions that were derived from inversely fitting different model set-up to the experimental data. As the simplified method of Schindler (1980) assumes a vertical linear contribution of the water contents and pressure heads over the sample, a problematic assumption for the relatively large soil samples of our study, some systematic error must be expected for the directly derived hydraulic properties. Nevertheless, the directly derived functions can serve as a reference for the inversely-derived functions. For some fitted set-ups, there is good agreement with directly derived hydraulic properties, especially for sample AK1. The different water retention functions of AK1 (Fig. 7a) show similar characteristics especially for the pressure head range between −50 cm and −500 cm. For higher pressure heads there are some discrepancies, which are mainly caused by the systematic error of the directly derived functions, due to the non-linear water content profile at the initial phase of the experiment. In the directly derived water retention function, the mean tensiometer value of 0 cm corresponds to a water level that is in the center of the soil sample. The upper part is already unsaturated, leading to an underestimation of the water contents at the initial pressure heads in the directly derived water retention functions. For the inverse estimation, θ_s was fixed to the value of the fully saturated sample.

The water retention characteristics for SF2 (Fig. 7c) are more variable than those of AK1. For the **full range**, the highest discrepancy to the directly derived retention function is indicated by the 4p model, which also showed high Φ values. For the 5p and 6p_d models the discrepancies get smaller with a good agreement between −70 cm and −500 cm. Looking at the **wet range**, the directly derived and inversely-fitted water retention functions match very well for the 6p_d model, even if the reduction of Φ

using a bimodal model was negligible. The 4p and 5p model set-ups fit well for pressure heads from −20 cm to −200 cm.

The hydraulic conductivity curves show a high variability for both shown samples (Fig. 7b and d). For the range of the directly derived unsaturated hydraulic conductivity (pressure heads < ∼−50), all curves for the *Sphagnum* peat (SF2), except for the 4p models, show similar characteristics. For AK1, the hydraulic conductivity curves from the models fitted to the full range have a better agreement with the directly derived curves than those fitted to the wet range only. This is consistent with the observation that stronger gradients only occurred under dry conditions in the full range and thus the shape parameter τ is only a sensitive parameter when fitting the full range.

The variability of the inversely-determined hydraulic properties raises the question which model set-up is best suited to simulate the unsaturated water flow in organic soils. Models are always characterized by some structural model error. When applying vGM-based models to organic soils, this error may be higher than for mineral soils given the specific characteristics of organic soils. In practice, the negative effect of this structural model error should be minimized as far as possible. Our results indicate that the model is not able to describe both the dry and wet range well with a single parameter set, thus, it is a practical solution to restrict the pressure head range during calibration to the most relevant range for specific applications and site conditions. Instead of restricting the range, individual weighting to specific ranges could also be introduced. Thus, if field measurements are available and if pressure heads do not fall below −200 cm for most times and parts of the soil, a reduction of the modeled pressure head range to 0 to −200 cm is advisable, or alternatively a method should be applied that gives higher weight on the wet range when fitting the full range. In contrast, if a good prediction of the actual evaporation rates from bare organic soil is intended (in our experiments the potential evaporation rate was pre-defined using the measured data), the calibration range should range to values much lower than −800 cm. For bare organic soils, the uppermost centimeters are supposed to fully dry out during dry periods. A specific consideration of such conditions is beyond the scope of this paper.

Results clearly indicated that the bimodal model that accounts for macropores is essential to achieve a good representation of the water content dynamics in the wet pressure head range. To simplify the bimodal macropore model of Durner (1994), the parameters α_2 and n_2 can be set to 1 and 10, which led to accurate results for all investigated organic soils in this study. For only one soil, the *Sphagnum* peat, the bimodal model did not seem to provide a major improvement. This soil is characterized with the highest fraction of macropores (35% of the pores are drained at pressure heads >−50 cm, see Fig. 7), but obviously the transition to smaller pores occurs rather continuously. A bi-modality is not apparent in the wet range, and thus, the wet range can be equally well described with an unimodal function.

If the pressure heads from field measurements fall below −200 cm, our results indicate that using the default value of $\tau = 0.5$ for mineral soils is not recommendable except for the degraded peat of GM with an organic carbon content of only 18%. According to this, the impact of τ increases from highly degraded to more natural pristine organic soils.

The results of this study indicate that the usage of hydraulic properties derived by classical laboratory measurements only (hanging water column and pressure plate for the water retention characteristic, constant- or falling head experiments for the saturated hydraulic conductivity) can lead to high model errors. The main problems are the fixed K_s values and the determination of parameter τ, which both result in an inaccurate unsaturated hydraulic conductivity function. Therefore, we recommend the use of dynamic experiments, such as evaporation or MSO experiments in combination with inverse optimization, to determine the hydraulic properties. If this is not possible, the macropore fraction should at least be determined from the experimentally derived retention curve and treated explicitly as a rapidly filling and emptying water reservoir when modeling the water dynamics in peat soils. In future, when data from more dynamic experiments with peat soils becomes available in literature, the derivation of default τ values for different peat soils may be also useful to improve the modeling when only parameters of classical methods are available. Applying the different hydraulic properties to reproduce measured tensiometer, water content and water level data in the field under transient conditions could provide more information about the most accurate way to model the water flow in organic soils.

4. Conclusions

The five different investigated organic soils of this study show contrasting properties and thus represent in part the broad variability of organic soils. The present study shows that the simulation of the unsaturated water flow in organic soils with the Richards' equation and vGM- and bimodal soil hydraulic models can lead to results of very variable quality. These single-domain models that were originally developed to model unsaturated flow in mineral soils are also frequently used to model hydrology of peatland areas. Our findings point out options to improve the performance of these simple models when they are applied to organic soils. We expect e.g. a better description of vertical moisture distribution profiles and water level fluctuations when considering these options.

For our evaporation experiments, the model performance depended on the model set-up (unimodal or bimodal vGM, fixing or optimizing certain parameters), and the peat type (botanical origin and degree of peat decomposition). When an adequate model set-up (our detailed recommendations are mentioned below) is chosen, modeled data fit the measured pressure heads and evaporation rates fairly well. Although organic soils have changing porosities during experiments due to shrinkage, and thus the physical basis of the Richards' equation is not fulfilled in terms of a rigid matrix, its application to peat soils seems to be a practical approach. However, the results also indicated that there is a weak trend towards better model performance for soils with higher degree of decomposition, and thus more rigid, mineral soil-like behavior.

However, we stress that these conclusions were drawn for dewatering conditions. For wetting conditions, in particular strong rainfall events, potential preferential and non-equilibrium flow cannot be described by the single-domain approach, especially when there are large macropores and cracks in the soil. Also hysteresis and hydrophobicity effects were not analyzed. Further experimental studies that are conducted under alternating flow directions are needed to evaluate model performance of single-domain approaches under the full range of natural boundary conditions.

Two major aspects need to be considered when modeling water flow in organic soils. Accounting for macropores is crucial and becomes apparent when focusing on the model performance of the wet pressure head range (here defined from 0 to −200 cm). A simplified bimodal model, with one additional fitting parameter that accounts only for the very large macropores, provided a much better representation of the measured pressure heads and evaporation rates than the unimodal model. Therefore, a practical approach for hydrological models is given and can also be realized on large scale applications under the limitation that preferential and non-equilibrium flow cannot be described by the single-domain Richards equation model used in the study.

When field pressure heads are expected to decrease below −200 cm for large parts of the soil profile, it is necessary to get an estimate of the vGM parameter τ, because results of this study indicated that τ from peat soils can strongly differ from the default value of 0.5 often used for mineral soils. As mentioned in Section 3.2 there is a necessity to describe a less steep decreasing hydraulic conductivity function than the one predicted by $\tau = 0.5$ which is shown by mostly negative optimized τ values. The negative τ values are partly able to describe the less steep decreasing conductivity function and lead for most of our simulations to a strong improvement of Φ. Using a different model, e.g. the one of Peters (2013) accounting for film and corner flow, would also lead to a less steep decreasing unsaturated hydraulic conductivity. Whether such a model is better suited to describe the observed unsaturated conductivity is beyond the scope of this paper.

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Appendix A. Supplementary material

Supplementary data associated with this article can be found, in the online version, at http://dx.doi.org/10.1016/j.jhydrol.2014.04.047.

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