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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

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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

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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;