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Jensen, J. L., Schjonning, P., Watts, C. W., Christensen, B. T. and Munkholm, L. J. 2018. Soil Water Retention: Uni-Modal Models of Pore-Size Distribution Neglect Impacts of Soil Management. *Soil Science Society of America Journal.* 83 (1), pp. 18-26.

Modelling Soil Water Retention: A Uni-modal Pore Size Distribution Does Not Reflect Reality

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ACKNOWLEDGEMENTS

The study was supported by the Green Development and Demonstration Programme (GUDP) of the Ministry of Environment and Food of Denmark (projects OptiPlant and OptiTill). The Rothamsted Long-term Experiments National Capability (grant code BBS/E/C00J0300) is supported by the UK Biotechnology and Biological Sciences Research Council (BBSRC) and the Lawes Agricultural Trust.

SUPPLEMENTAL MATERIAL

Supplemental material is available with the online version of this article. The supplemental document presents parameter estimates of the van Genuchten and double-exponential model for the 16 Danish top- and subsoils of the Jakobsen data set and the 16 plots at Highfield.

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Abstract (It is 1683 characters incl. spaces □ should be max 1500)

Reliable models for describing soil water retention are vital when simulating plant production and environmental effects in agroecosystems. Models for describing soil water retention often imply a uni-modal pore size distribution (PSD) such as the one suggested by van Genucthen (vanG). However, clear deviations from a uni-modal PSD has been documented. The double-exponential (Dex) model imply a bi-modal PSD and may better reflect reality. We evaluated how the vanG and Dex models fit to water retention data for top- and subsoil differing in texture, soil with contrasting management systems (Highfield), and a soil with different tillage practices (Flakkebjerg). Soils were subjected to matric potentials from -10 hPa to -1.5 MPa using conventional methods. The bi-modal Dex model provided a better fit to water retention data for relatively sandy top- and subsoil, and the contrasting treatments from Highfield and Flakkebjerg, than the uni-modal vanG model. Neither of the models worked well for highly sorted soils. Topsoil was less well described than subsoil when using the vanG model due to a more pronounced bi-modality of the PSD caused by increased soil organic carbon (SOC) content and tillage. The root mean square error of the vanG fit increased with an increase in SOC when going from the bare fallow to the grass treatment at Highfield. At the same time, the tillage intensity decreased, but the effect of SOC seemed to outweigh the lack of tillage. These observations were reflected in a more distinct bi-modality of the PSD for better structured soils. Consequently, we suggest that uni-modal models are too simplistic for describing management effects on PSD.

Abbreviations: AIC, Akaike's information criterion; C, capacity; d_2, dominating pore size of the structural peak; Dex, double-exponential; I, intensity; PSD, pore size distribution; Q, quantity; RMSE, root mean squared error; SOC, soil organic carbon; SOM, soil organic matter; V_1, textural void ratio; V_2, structural void ratio; vanG, van Genuchten; VIF, variance inflation factor.

Core Ideas (3-5; 85 characters with spaces)

- A uni- and a bi-modal soil water retention model were evaluated
- The bi-modal double-exponential model provided a better fit
- The uni-modal model fit was affected by texture, soil organic carbon and tillage
- Uni-modal models cannot accurately describe the pore size distribution

Keywords (at least 2): Pore size distribution; Soil water retention.

Soil water and air is crucial for plant growth, microbial activity and percolation (Rabot et al., 2018). Consequently, quantitative knowledge of the pore size distribution (PSD) is essential. As a result, reliable models for describing soil water retention are vital when simulating water and solute movement, plant growth, and microbial driven processes such as carbon turnover and denitrification.

Soil water can be described in terms of quantity (Q, e.g. volumetric water content) and intensity (I, e.g. matric potential). Consequently, Q at any I is the volumetric water content retained in all pore size classes smaller than that defined by I. The ratio of Q and I at any given I is then the capacity (C), providing a measure of the volume of pores for a given tube-equivalent pore size. Numerous models for describing soil water retention has been suggested, and the most widely used are uni-modal analytical expressions (Cornelis et al., 2005) such as the one proposed by Brooks and Corey (1964).

van Genuchten (1980) suggested the most widely used model for describing soil water retention (>10000 citations; Web of Science, May 2018). The fitting parameters of the van Genuchten (vanG) model are often used to indirectly determine the unsaturated hydraulic conductivity of a soil (Mualem, 1986), and many pedotransfer functions have been developed for predicting the vanG parameters based on basic soil properties (Cornelis et al., 2001; Minasny et al., 1999; Patil and Singh, 2016). The unsaturated hydraulic conductivity predicted by the vanG parameters are often used as input in simulation models such as Daisy (Hansen et al., 2012) and HYDRUS (Šimunek et al., 2012). The simulations are used to predict plant production and environmental effects and may be used as basis for political decision-making.

Also, the vanG model implies a uni-modal PSD. Uni-modal models implicitly assumes a maximum C at one specific I (corresponding to a specific pore size). However, presenting the size distribution of pores by frequency, by for example numerical differentiation of the Q/I curve, has documented clear and important deviations from a uni-modal PSD (Eden et al., 2011; Pulido-Moncada et al., 2018; Schjønning, 1992). This calls for a more flexible description of the pore system than that obtained by uni-modal expressions. Several non-uni-modal models have been proposed (e.g, Poulsen et al., 2006; Ross and Smettem, 1993). Dexter et al. (2008) proposed a double-exponential model (Dex), which describes bi-modal PSD, i.e. a size distribution of pores with two peaks. The two peaks are denoted textural and structural pore spaces, and the division is based on a mechanistic understanding of soil structure (Dexter, 1988; Dexter et al., 2008). Thus, the Dex model may be one way of trying to allow for a better description of reality. Further, the Dex model has the additional advantage in providing parameters with physical meaning when compared to the vanG model.

The objective of this study was to evaluate how the uni-modal vanG and bi-modal Dex model fit to water retention data for 1) top- and subsoil with different texture, 2) soil with contrasting long-term crop rotations, and 3) a soil subject to different tillage practices.

MATERIALS AND METHODS

The Jakobsen data set

A PhD-study focused on the hydraulic properties of 16 contrasting soils distributed throughout Denmark, each with sampling done in the top- (~0.10 m) and subsoil (~ 0.50 m) layers (Jakobsen, 1989). The topsoil ranged from loamy sand to silt loam with the main part being sandy loam or loam soils. The Jyndevad and Tylstrup soils were extremely sorted with 51.2 g 100 g^{-1} minerals in the 200-500 µm fraction and 51.8 g 100 g^{-1} minerals in the 63-125 μm fraction, respectively. The soil textural composition of top- and subsoil can be seen in Table 1 and 2, respectively.

Table 1. Soil textural composition and organic carbon (SOC) content in the ~0.10 m layer of the 16 Danish soils of the Jakobsen (1989) data set listed in order of increasing clay content. The Rosin-Rammler parameters (α and β) were calculated by Eq. 6 and are based on the seven particle size fractions listed in Jakobsen (1989).

Site	SOC	Clay, <2 μm	Silt, 2-20 μm	Silt, 20-63 μm	Sand, 63-2000 μm	α	β
	(g 100 g^{-1} minerals)					(μm)	-
Hals	2.36	2.6	3.4	7.9	86.0	150	1.76
Tylstrup	1.30	3.7	4.9	17.2	74.2	88	3.58
Jyndevad	1.36	4.2	3.9	3.2	88.8	367	1.41
Borris	1.31	5.7	7.8	22.8	63.7	131	0.96
Hornum	1.86	5.8	8.4	13.3	72.5	180	0.93
Travsted	3.38	7.7	6.8	16.2	69.3	189	0.86
Foulum	1.49	7.9	10.1	15.6	66.4	176	0.75
Ødum	1.49	10.1	15.5	20.2	54.3	104	0.71
Årslev	1.36	10.6	14.9	21.1	53.4	95	0.79
Roskilde	1.43	10.8	17.3	19.3	52.7	93	0.74
Askov	1.55	11.0	12.6	16.5	59.9	124	0.77
Rønhave	1.24	14.5	15.6	27.5	42.4	65	0.78
Tystofte	1.18	14.7	16.4	19.5	49.4	75	0.73
Ø. Ulslev	1.38	15.8	15.5	16.5	52.2	102	0.58
Kalø	0.82	17.7	14.4	15.9	52.0	102	0.55
Højer	1.73	18.6	15.4	39.9	26.0	42	1.00

Table 2. Soil textural composition and organic carbon (SOC) content in the ~0.50 m layer of the 16 Danish soils of the Jakobsen (1989) data set listed as in Table 1. The Rosin-Rammler parameters (α and β) were calculated by Eq. 6 and are based on the seven particle size fractions listed in Jakobsen (1989).

Site	SOC	Clay, <2 μm	Silt, 2-20 μm	Silt, 20-63 μm	Sand, 63-2000 μm	α	β
	(g 100 g^{-1} minerals)					(μm)	-
Hals	0.17	2.0	0.5	1.0	96.5	190	3.31
Tylstrup	0.29	3.1	2.4	12.8	81.7	82	5.96
Jyndevad	0.35	3.5	1.9	1.0	93.6	359	2.25

Borris	0.29	11.2	7.3	14.9	66.6	136	0.90
Hornum	0.17	7.2	6.3	13.7	72.8	200	0.88
Travsted	0.35	10.8	6.7	10.8	71.7	194	0.84
Foulum	0.17	13.4	9.6	13.4	63.5	166	0.64
Ødum	0.17	16.5	12.6	16.4	54.4	106	0.60
Årslev	0.17	20.4	12.6	15.9	51.0	78	0.63
Roskilde	0.29	23.8	16.3	11.9	48.0	72	0.49
Askov	0.35	24.5	11.6	14.3	49.6	72	0.55
Rønhave	0.29	19.6	16.5	25.1	38.8	53	0.67
Tystofte	0.29	22.8	15.3	17.9	44.0	58	0.58
Ø. Ulslev	0.23	15.6	13.5	14.1	56.8	120	0.59
Kalø	0.29	26.8	12.4	14.3	46.6	77	0.43
Højer	0.24	7.9	6.4	35.6	50.1	69	3.08

The soils were all long-term arable and derived from the Weichsel glacial stage (glacial deposits: ten soils; glaciofluvial deposits: Jyndevad), the Saale glacial stage (glacial deposits: Borris and Travsted), the raised Holocene sea floor (Tylstrup and Hals), and one soil present-day marine marsh area (Højer).

At each site, topsoil was sampled in six plots of about one m^2, whereas subsoil was sampled in one of these plots. In the topsoil, three 100 cm^3 soil cores (61 mm diameter, 34 mm height) were sampled in each plot providing 18 cores pr. site. In the subsoil, nine cores were sampled at each site.

Rothamsted Highfield ley-arable experiment

Data on soil texture, soil organic carbon (SOC) and pore characteristics for the Highfield long-term ley-arable experiment at Rothamsted Research, UK (51°80’N, 00°36’W) was recently published by Jensen et al. (2018) and Obour et al. (2018). In this study, we use these data for four treatments: Bare fallow maintained free of plants by regular tillage since 1959, Continuous arable rotation with winter cereals since 1948, Ley-arable rotation; a three-year grass-clover ley followed three years arable since 1948, and grass, grassland ploughed and reseeded to grass in 1948. The bare fallow treatment was cultivated three to five times per year, arable once a year, ley-arable once in two years (in six-year cycle) and grass had not been cultivated since 1947. The arable, ley-arable and grass treatments were embedded in a randomized block design, whereas the bare fallow plots were not part of the original design and located at one end of the experiment. The soil type is silt loam and is classified as Aquic Paleudalf (USDA Soil Taxonomy System). The parent material includes a silty (loess-containing) deposit overlying and mixed with clay-with-flints (Avery and Catt, 1995).

Soil was sampled in spring 2015. Six 100 cm^3 soil cores (61 mm diameter, 34 mm height) were extracted from the ~0.10 m soil layer of each of a total of four plots providing 24 cores per treatment. More details are given in Jensen et al. (2018) and Obour et al. (2018).

Flakkebjerg tillage experiment

Previously published data on SOC and pore characteristics for the long-term experiment on conservation tillage at the Flakkebjerg experimental site in Denmark (55°19’N, 11°23’E) was used. Treatments kept under moldboard plowing to 0.20-m depth and direct drilling were compared after eleven years of different tillage practices. The treatments were embedded in a split-plot experiment with four replicates. The soil type is a sandy loam soil with 14.7 % clay (<2 µm), 13.7 % silt (2-20 µm), 42.6 % fine sand (20-200 µm) and 27% coarse sand (200-2000 µm). The soil is classified as Oxyaquic Agriudoll (USDA Soil Taxonomy System). The rotation included winter and spring crops (mainly cereals) with residues removed.

Soil was sampled in autumn 2013. Six 100 cm^3 soil cores (61 mm diameter, 34 mm height) were extracted from the 0.12-0.16 m soil layer of each plot providing 24 cores pr. treatment. Further details can be found in Abdollahi and Munkholm (2017).

Laboratory measurements

Soil texture was determined on air dry bulk soil (<2-mm) with a combined hydrometer/sieve method (Gee and Or, 2002). Samples from Highfield were treated with hydrogen peroxide to remove soil organic matter (SOM), while this was not done for Flakkebjerg and the Jakobsen soils. The content of SOC was measured by dry combustion using a Thermo Flash 2000 NC Soil Analyser (Thermo Fisher Scientific, Waltham MA, USA) for Highfield and Flakkebjerg, and a LECO CNS-1000 analyzer (LECO Corporation, St. Joseph, MI) for the Jakobsen soils.

Before measuring soil water retention, the soil cores were placed on the top of a tension table to be saturated from beneath. For the Jakobsen data set, soil water retention was measured at -4 (Højer only), -10, -16, -50, -100, -160 and -500 hPa matric potential, and at -10, -30, -100, -300 and -1000 hPa matric potential for Highfield and Flakkebjerg using tension tables and pressure plates (Dane and Hopmans, 2002). The soil cores were oven-dried (105 °C for 24 h), and bulk density calculated. For Highfield, bulk density was corrected for stone weight and volume because the soil contained a significant amount of stones. Soil porosity was estimated from bulk density and particle density. Particle density was measured by the pycnometer method (Flint and Flint, 2002). For Highfield, particle density was measured on one plot from each treatment, and the particle density for the remaining plots were predicted from SOC by a linear regression model. For Flakkebjerg, a particle density of 2.65 g cm^{-3} was used based on previous studies (Abdollahi and Munkholm, 2017).

Water retention at -1.5 MPa was determined on <2-mm air-dry soil for each site and depth for the Jakobsen soils and at plot level for Highfield. For the Jakobsen and Highfield soils a pressure plate system and a WP4-T Dewpoint Potentiometer, respectively, was used (Scanlon et al., 2002). For Flakkebjerg, water retention at -1.5 MPa was predicted based on clay and SOC content using Eq. 1 in Hansen (1976).

Pore water suction was assumed to relate to an average pore size by the approximate relation:

$d = -3000/h$ [1]

where d is the tube-equivalent pore diameter (µm) and h is the soil matric potential (hPa).

Soil water retention models

The water retention data was fitted to the van Genuchten (1980) model (termed vanG):

$$\theta = (\theta_{\text{sat}} - \theta_{\text{res}})\left[1 + (\alpha h)^n\right]^{-m} + \theta_{\text{res}} \quad [2]$$

where $\square_{\text{sat}}$ and $\square_{\text{res}}$ are the water contents at saturation and the residual water content, respectively, h is the soil matric potential, α is a scaling factor for h and n and m are parameters that control the shape of the curve. The widely used Mualem (1976) restriction ($m = 1\text{-}1/n$) was used to prevent over-parametrization (Dexter et al., 2008) and unstable results (van Genuchten et al., 1991). The Mualem restriction is also recommended, when only measured values in the wet range are used (van Genuchten et al., 1991). The PSD predicted by the vanG model was obtained by differentiating Eq. 2 with respect to matric potential:

$$\frac{d\theta}{d(\log_{10} h)} = (\theta_{\text{sat}} - \theta_{\text{res}})(\alpha n(\alpha h)^{n-1}(-m)(1 + (\alpha h)^n)^{-m-1})h \ln 10 \quad [3]$$

The double-exponential model proposed by Dexter et al. (2008) was fitted to water retention data (termed Dex):

$$\theta = C + A_1 e^{(-h/h_1)} + A_2 e^{(-h/h_2)} \quad [4]$$

where C is the residual water content, A_1 and A_2 are the amount of textural and structural pore space, respectively, and h_1 and h_2 are the characteristic pore water suctions at which the textural and structural pore spaces empty, respectively. The PSD predicted by the Dex model was obtained by differentiating Eq. 4 with respect to matric potential:

$$\frac{d\theta}{d(\log_{10}h)} = -\frac{A_1}{h_1}e^{(-h/h_1)}h\ln 10 - \frac{A_2}{h_2}e^{(-h/h_2)}h\ln 10 \quad [5]$$

The parameters of the vanG model were obtained using the curve-fitting program RETC (van Genuchten et al., 1991), which is based on a nonlinear least-squares optimization approach. Similarly, the parameters of the Dex model were obtained by nonlinear regression analysis to achieve the smallest residual sum of squares.

Calculations and statistics

The Rosin-Rammler equation (Eq. 2 in Rosin and Rammler (1933)) was fitted to the seven chemically dispersed particle size fraction listed in Jakobsen (1989), i.e. <2, 2-20, 20-63, 63-125, 125-200, 200-500 and 500-2000 µm, for each soil. It can be written as:

$$P(X < x) = 1 - \exp\left(-\left(\frac{x}{\alpha}\right)^{\beta}\right) \quad [6]$$

where $P(X<x)$ is the fraction by weight of particles less than size x, α indicates the coarseness of particles and β indicates the spread of particle sizes. Eq. 6 described the particle size distribution of the soils well, with coefficients of determination (R^2) from 0.95 to 1.00.

For the statistical analysis, the R-project software package Version 3.4.0 (R Foundation for Statistical Computing) was used. Treatment effects for Highfield was analyzed as described in Jensen et al. (2018). The key indices of goodness of fit were Akaike’s information criterion (AIC), which was used to compare models with different number of parameters (Akaike, 1973), and the root mean squared error (RMSE):

$$\mathrm{RMSE} = \sqrt{\frac{1}{N}\sum(\theta_{\mathrm{meas}} - \theta_{\mathrm{fitted}})^2} \quad [7]$$

where N is the number of matric potentials. Multiple linear regression was used to identify how structural void ratio (V_2) related to SOC, soil texture and void ratio. Structural void ratio was calculated as follows: $V_2 = A_2 / (1-P)$, where A_2 is the Dex model estimate of structural pore space, and P is porosity. Likewise, textural void ratio (V_1) was calculated. The variance inflation factor (VIF) was calculated when more than one predictor was used in the regression. The VIF expresses the degree of multicollinearity among the predictors. Upper value limits of VIF for non-erroneous conclusions from multiple regressions has been set to five (Rogerson, 2001) or ten (Kutner et al., 2004).

RESULTS

Jakobsen data set

The soils differed in their textural composition and SOC content (Tables 1 and 2). In the topsoil, clay ranged from 2.6 to 18.6 g 100 g^{-1} minerals and SOC from 0.82 to 3.38 g 100 g^{-1} minerals, whereas the range in the subsoil was from 2.0 to 26.8 g clay 100 g^{-1} minerals and from 0.17 to 0.35 g SOC 100 g^{-1} minerals. The α-parameter for topsoil ranged from 42 to 367 µm and for subsoil from 53 to 359 µm. The Jyndevad soil, however, stand out being very coarse textured ($\alpha_{\mathrm{topsoil}}$=367 µm, $\alpha_{\mathrm{subsoil}}$=359 µm), and the range changed to 42 to 200 µm if omitting Jyndevad. The β-parameter describes the spread of particle sizes, with large values indicating that the soil is well sorted (a narrow range of particle sizes), and small values indicating that the soil is graded with an evenly distributed mass of particles in all size classes. The β-parameter for topsoil ranged from 0.55 to 3.58 and for subsoil from 0.43 to

5.96. The twelve glacial till soils, however, had a narrow range from 0.43 to 0.96, whereas Hals, Tylstrup, Jyndevad and Højer were highly sorted with β>1 (Tables 1 and 2).

Mean AIC and RMSE values, when using the vanG and Dex models were calculated for the top- and subsoil. For topsoil, values of AIC were -58.6 and -70.6 and RMSE were 0.011 and 0.005 $m^3\,m^{-3}$ using vanG and Dex, respectively. For subsoil, values of AIC were -63.2 and -75.1 and RMSE were 0.008 and 0.005 $m^3\,m^{-3}$. However, the four highly sorted soils (β>1) had relatively poor goodness of fit measures both when using the vanG and Dex models (Fig. 1, Tables S1 and S2).

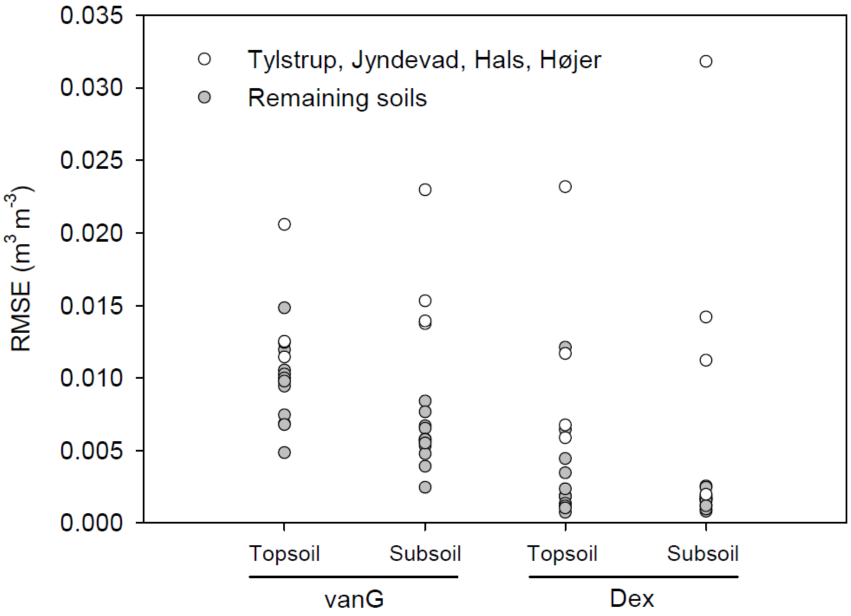

Fig. 1. The root mean squared error (RMSE) value for the Danish top- and subsoil of the Jakobsen data set using the van Genucthen (vanG) or double-exponential (Dex) model.

If the highly sorted soils are omitted in the calculation of the mean AIC and RMSE values, the vanG model gives AIC values of -59.6 and -66.8 and RMSE values of 0.009 and 0.006 $m^3\,m^{-3}$ in top- and subsoil, respectively. The Dex model gives AIC values of -75.1 and -80.9 and RMSE values of 0.003 and 0.002 $m^3\,m^{-3}$ in top- and subsoil, respectively. The lower AIC and

RMSE values obtained for the Dex compared to the vanG model indicate a better ability to describe data.

We tested the correlation between the structural void ratio (V_2) and the variables α, β, void ratio, SOC and clay content. This was done for both top- and subsoils and with and without exclusion of the highly sorted soils (β>1). For topsoil samples V_2 could be well predicted by log(β) and clay content:

$$V_2 = 0.558^{***}(\pm 0.118) \times \log(\beta) - 0.011^{*}(\pm 0.005) \times \text{clay} + 0.424^{***}(\pm 0.048),$$

$$s=0.068,\ R^2=0.84 \quad [8]$$

Excluding the highly sorted samples from topsoil gave:

$$V_2 = 0.878^{***}(\pm 0.143) \times \beta - 0.441^{**}(\pm 0.110),\ s=0.057,\ R^2=0.79 \quad [9]$$

For subsoil samples V_2 could be well predicted by log(β) and α:

$$V_2 = 0.592^{***}(\pm 0.078) \times \log(\beta) - 0.001^{**}(\pm 0.0003) \times \alpha + 0.184^{**}(\pm 0.050),$$

$$s=0.100,\ R^2=0.85 \quad [10]$$

Excluding the highly sorted samples from subsoil gave:

$$V_2 = 0.289^{***}(\pm 0.025) \times \beta,\ s=0.057,\ R^2=0.55 \quad [11]$$

In Eq. 8-11, the numbers in parentheses are standard errors of estimate, and s is the standard deviation of the predicted value. When developing the four models, we tested for multicollinearity and interaction among the predictors, but only low VIF values and no significant interactions were found.

Rothamsted Highfield ley-arable experiment

The soils at Highfield ranged from 0.84 to 4.04 g SOC 100 g^{-1} minerals and soil texture was in general not significantly different between treatments (Table 3).

Table 3. Soil textural composition and organic carbon (SOC) content of the four treatments from Highfield. Within rows, letters denote statistical significance at $P<0.05$ for the comparison of Arable, Ley-arable and Grass. An asterisk (*) indicates if Bare fallow is significantly different from the other treatments based on a pairwise *t*-test. Data from Jensen et al. (2018).

Treatment	SOC	Clay, <2 µm	Silt, 2-20 µm	Silt, 20-63 µm	Sand, 63-2000 µm
	(g 100 g^{-1} minerals)				
Bare fallow	0.90	27.0	24.9	33.5	14.6
Arable	1.73a*	26.4	26.3	31.8	15.5
Ley-arable	2.16a*	25.5	26.1	32.4	16.0
Grass	3.29b*	26.1	27.2*	31.9	14.8

Thus, the effect of contrasting long-term management could be investigated without confounding effects related to variations in soil type. The Dex model generally fitted the water retention data for the contrasting treatments well (Fig. 2a).

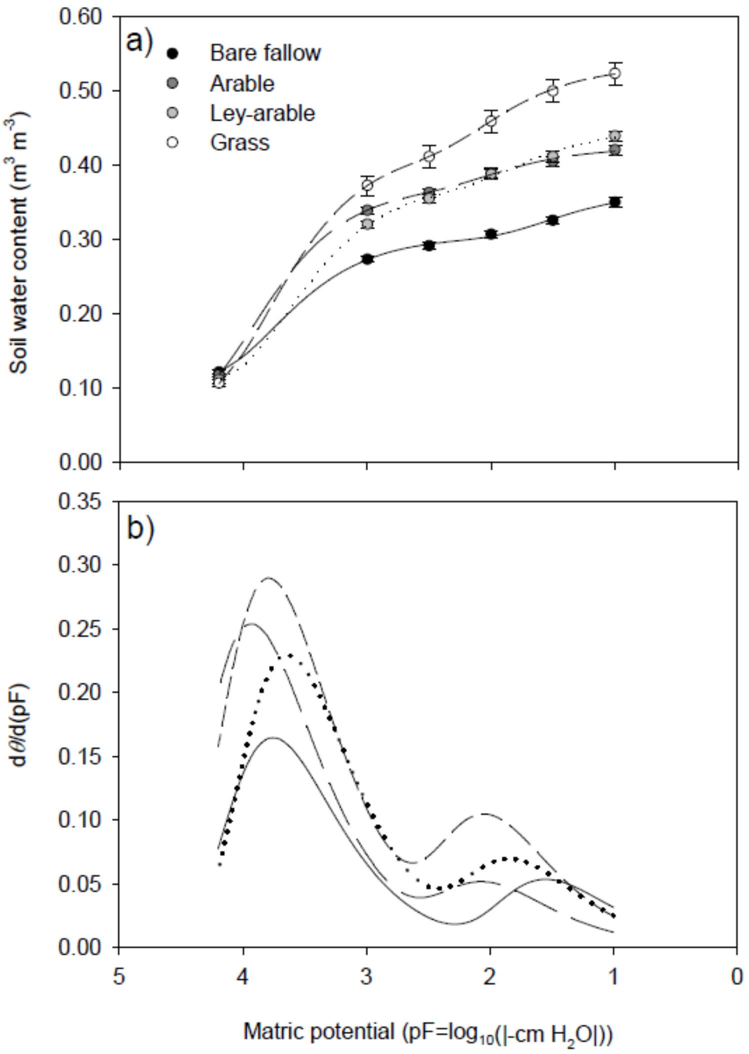

Fig. 2. (a) Measured volumetric water content for the four treatments at Highfield and fits of the double-exponential (Dex) model as a function of matric potential. The standard error of the mean are indicated (*n*=4). **(b)** Pore size distribution (d□/d(pF)) as a function of matric potential for the four treatments. Eq. 5 was used to obtain the pore size distributions.

Mean values of AIC, when using the vanG and Dex models were -43.8 and -69.1, respectively. Similarly, mean values of RMSE were larger when using the vanG compared to the Dex model with values of 0.016 and 0.002 m^3 m^{-3}, respectively. The RMSE when using the vanG model increased from 0.010 to 0.028 m^3 m^{-3} with an increase in SOC from 0.84 to 4.04 g 100 g^{-1} minerals (Fig. 3), whereas no systematic error was observed when using the

Dex model (P=0.532). Parameter estimates and goodness of fit measures for the 16 individual plots can be seen in Table S3.

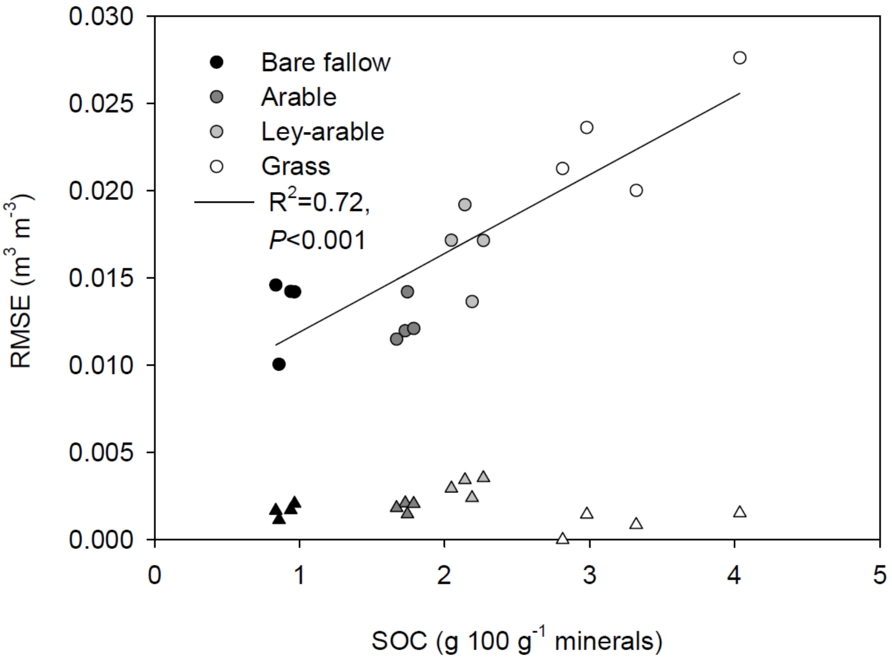

Fig. 3. The root mean squared error (RMSE) value as a function of soil organic carbon (SOC) for the four treatments at Highfield using the van Genucthen (vanG) model (circle symbols) and the double-exponential (Dex) model (triangle symbols).

Textural (V_1) and structural void ratio (V_2) increased with increasing SOC content and decreasing tillage intensity (V_1: R^2=0.91, P<0.001, V_2: R^2=0.74, P<0.001). The dominating pore size of the structural peak (d_2) was estimated to 86 µm for the bare fallow treatment, whereas it was significantly lower for the arable and grass treatments, and in between for ley-arable treatment (Table 4).

Table 4. Estimated parameters of the double-exponential model (Dex) of the four treatments from Highfield. Within rows, letters denote statistical significance at P<0.05 for the comparison of Arable, Ley-arable and Grass. An asterisk (*) indicates if Bare fallow is

significantly different from the other treatments based on a pairwise *t*-test. d_1 and d_2 indicate the dominating pore size of the textural and structural peak, respectively, and were estimated by Eq. 1.

	Parameters of the Dex model						
Treatment	C	A_1	h_1	d_1	A_2	h_2	d_2
	($m^3 m^{-3}$)	($m^3 m^{-3}$)	(hPa)	(µm)	($m^3 m^{-3}$)	(hPa)	(µm)
Bare fallow	0.110	0.195	5729	0.5	0.061	35	86
Arable	0.068a*	0.305ab*	8707b*	0.3	0.051a	97b*	31
Ley-arable	0.104b	0.271a*	4379a	0.7	0.073a	63a	48
Grass	0.080ab*	0.345b*	6216a	0.5	0.110b*	102b*	29

Flakkebjerg tillage experiment

Moldboard plowing to 0.20-m depth and direct drilling had contents of 1.25 and 1.08 g SOC 100 g^{-1} minerals, respectively, in the 0.12-0.16 m layer. The Dex model fitted the two treatments well (Fig. 4), and better compared to the vanG model as revealed by lower AIC and RMSE values (Plowing: AIC_{vanG}=-53.8 and AIC_{Dex}=-58.5, $RMSE_{vanG}$=0.006 $m^3 m^{-3}$ and $RMSE_{Dex}$=0.003 $m^3 m^{-3}$; Direct drilling: AIC_{vanG}=-62.5 and AIC_{Dex}=-69.3, $RMSE_{vanG}$=0.003 $m^3 m^{-3}$ and $RMSE_{Dex}$=0.001 $m^3 m^{-3}$).

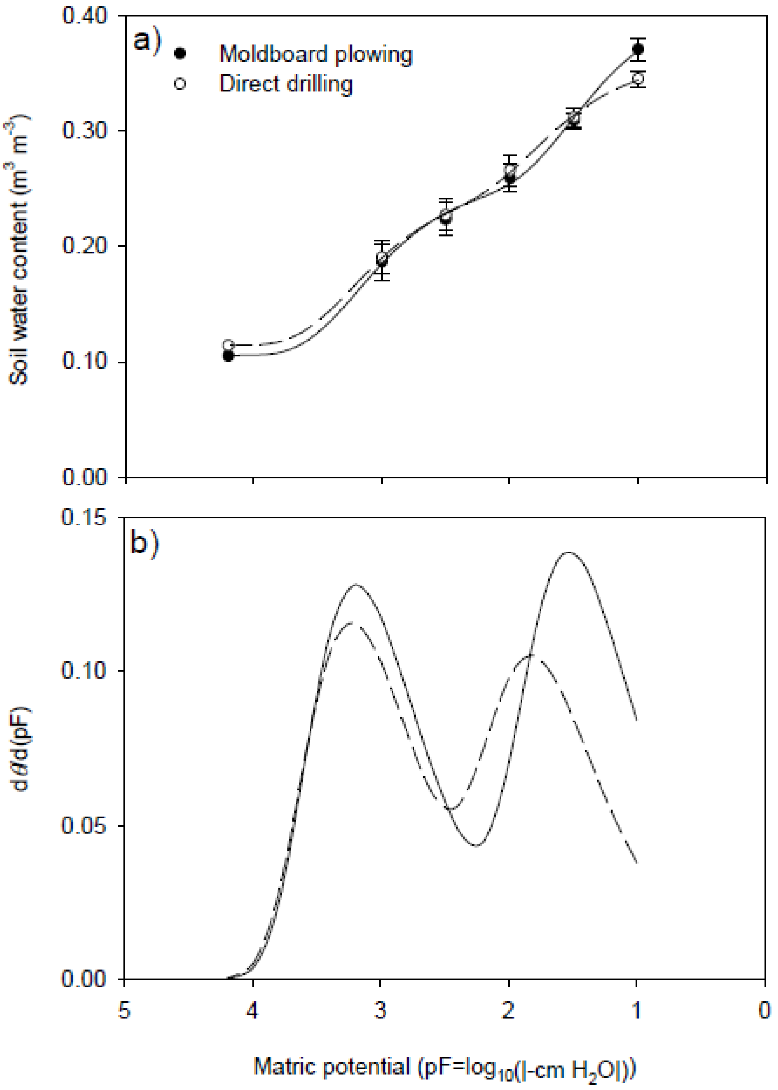

Fig. 4. (a) Measured volumetric water content for moldboard plowing to 0.20-m depth and direct drilling and fits of the double-exponential (Dex) model as a function of matric potential. The standard error of the mean are indicated (*n*=4), except for pF 4.2 which is predicted based on Eq. 1 in Hansen (1976). **(b)** Pore size distribution (d□/d(pF)) as a function of matric potential for the two treatments. Eq. 5 was used to obtain the pore size distributions.

Structural void ratio (V_2) for moldboard plowing and direct drilling was 0.30 and 0.19, respectively. The dominating pore size of the structural peak (d_2) was 50 µm for direct drilling and 94 µm for moldboard plowing.

DISCUSSION

Model fit

The Dex model provided a better fit to soil water retention data than the vanG model for the Jakobsen glacial till top- and subsoils. The same was the case for the contrasting treatments from Highfield and Flakkebjerg. Thus, the PSD for these soils was better described with a bi- rather than a uni-modal model. Also, Schjønning (1992) observed that the vanG model was not able to describe a general pattern of a double-peak PSD for glacial till soils. Similarly, Dexter et al. (2008) and Berisso et al. (2012) found that the Dex model fitted their data better than the vanG model. Dexter et al. (2008) based their analysis on 42 Polish soils (26 topsoils, six samples from 0.30-0.35 m depth and ten subsoils) ranging from 2 to 25 g clay 100 g^{-1}, whereas the study by Berisso et al. (2012) focused on a sandy clay loam ranging from 19 to 27 g clay 100 g^{-1}. Our study included soils ranging in clay content from 2.0 to 30.0 g 100 g^{-1} minerals substantiating that the Dex model is superior for soils <30 g clay 100 g^{-1} minerals. In summary, uni-modal models seem too simplistic for describing the size distribution of pores in most soils with less than 30 g clay 100 g^{-1} minerals.

Neither of the models worked well for highly sorted soils (β>1). This finding calls for alternative water retention models for soils with a narrow distribution of pore sizes. Dexter et al. (2008) mentioned the problems associated with the use of the Dex model for uniform sands. However, we emphasize that the Dex as well as the vanG model cannot describe highly sorted soils well regardless of the dominating particle size.

Pitfalls using uni-modal models – effects of soil organic carbon and tillage

The topsoil of the Jakobsen data set were less well described with the vanG model than the subsoil (Fig. 1). This could be ascribed to a more distinct bi-modal PSD for topsoil, which can be interpreted as a combination of larger SOC content and the presence of tillage (Fig. 5).

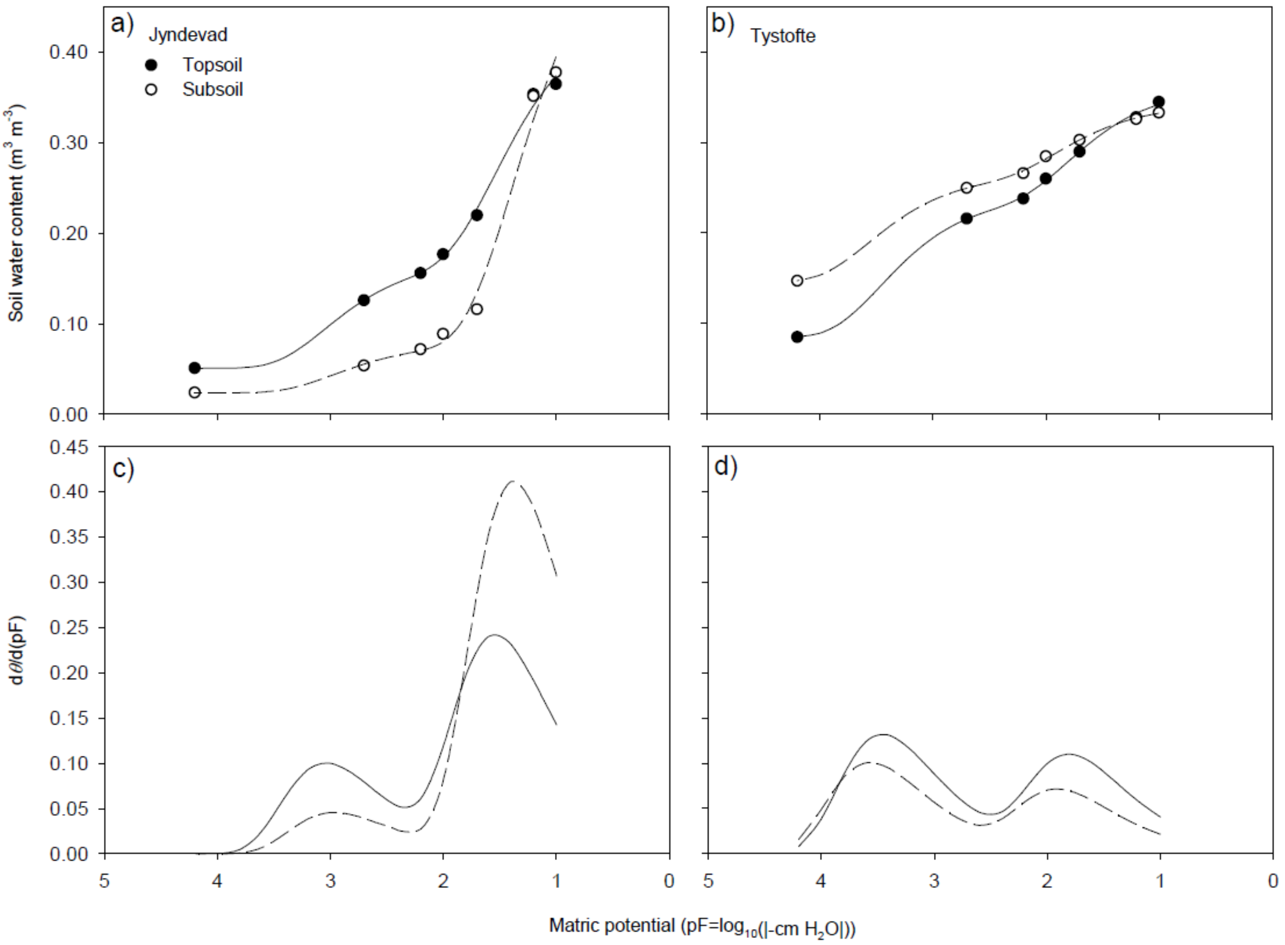

Fig. 5. (a, b) Measured volumetric water content for Jyndevad and Tystofte top- and subsoils of the Jakobsen data set and fits of the double-exponential (Dex) model as a function of matric potential. **(c, d)** Pore size distribution (d□/d(pF)) as a function of matric potential for Jyndevad and Tystofte top- and subsoils. Eq. 5 was used to obtain the pore size distributions.

Tillage increases the amount of large structural pores, and the effect of structure forming agents in subsoil are much reduced, which limits structural pore space at depth. Similarly, the systematic increase in RMSE with increasing SOC content for Highfield (Fig. 3) could be ascribed to a more pronounced bi-modal behaviour (Fig. 2b), most clearly seen for the grass treatment (Fig. 6).

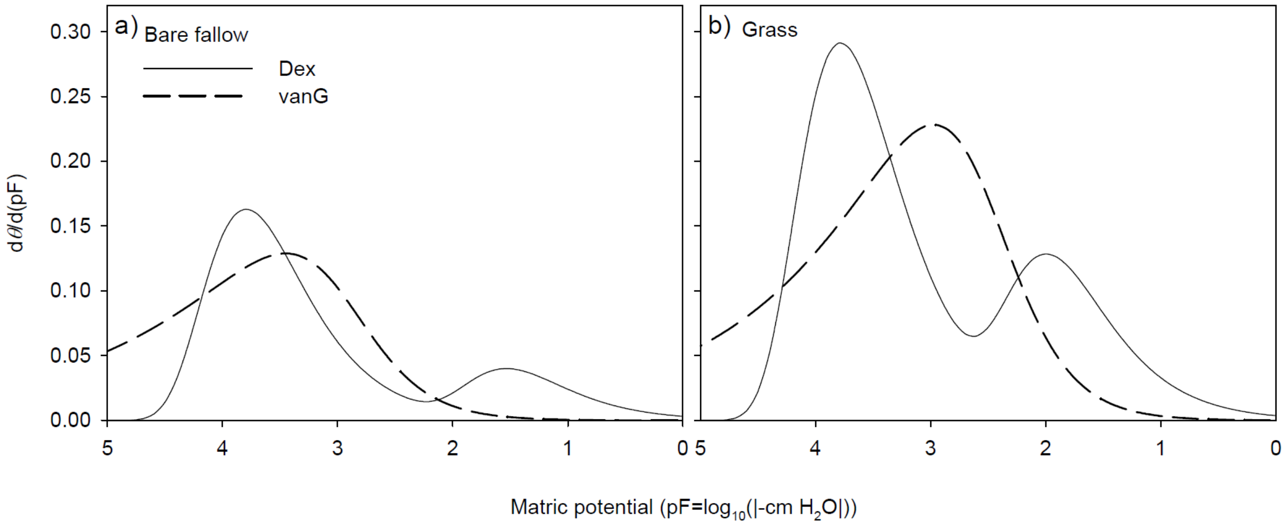

Fig. 6. Pore size distribution (d□/d(pF)) as a function of matric potential for **(a)** the bare fallow and **(b)** the grass treatment at Highfield either obtained by Eq. 5 for the double-exponential (Dex) model (solid line) or Eq. 3 for the van Genuchten (vanG) model (dashed line).

Soil organic carbon content may increase the textural pore space especially in soils with less than 19 g clay 100 g^{-1} (Rawls et al., 2003) due to its absorptive capacity for water. The structural pore space is mainly affected by SOC through improved aggregation (Bronick and Lal, 2005). Both V_1 and V_2 were positively affected by SOC at Highfield. However, the estimate of the mean size of structural voids (d_2) decreased with SOC. For Flakkebjerg, where plowing was compared to direct drilling, both V_2 and d_2 increased with tillage intensity. The limited effect of tillage on V_2 when going from the grass to the bare fallow treatment at Highfield suggests that the improving effect of SOC on soil structure outweighed any effect of tillage for these long-term treatments. Interestingly, d_2 was larger for the bare fallow than the grass treatment indicating that large pores were introduced by tillage as seen in Flakkebjerg.

Structural void ratio

The structural void ratio (V_2) is an important parameter for soil functioning such as air exchange and water uptake by plants. We used V_2 rather than volumetric water content in order to allow a comparison across soils with varying bulk density. From the previous section, we found that SOC content and tillage intensity were important drivers for V_2. In addition, soil texture affects V_2 through a positive relation to β (Eq. 8 to 11) indicating that the more sorted soils have larger V_2 than graded soils. This is in agreement with Ehlers and Claupein (1994), who reported that graded coarse textured soils readily compact to high densities. Similarly, Schjønning and Thomsen (2013) found that graded soils low in SOC showed a hard-setting behavior. A low V_2 may reduce soil aeration and potentially affect root growth and air exchange processes in a negative direction. Therefore, specific management strategies should be targeted on graded soil low in SOC, e.g. SOM promoting management.

Implications

Predicting water retention using the vanG model induced a larger error in top- than subsoil. Consequently, modelling whole profile water flow may be systematically biased down through the soil profile. For Highfield, the vanG model overestimated the pore volume in the size range 10-30 µm (pF 2.5-2) and underestimated the pore volume at pF 3 and 1. The error was more pronounced for the more structured grass than bare fallow soil (Fig. 7).

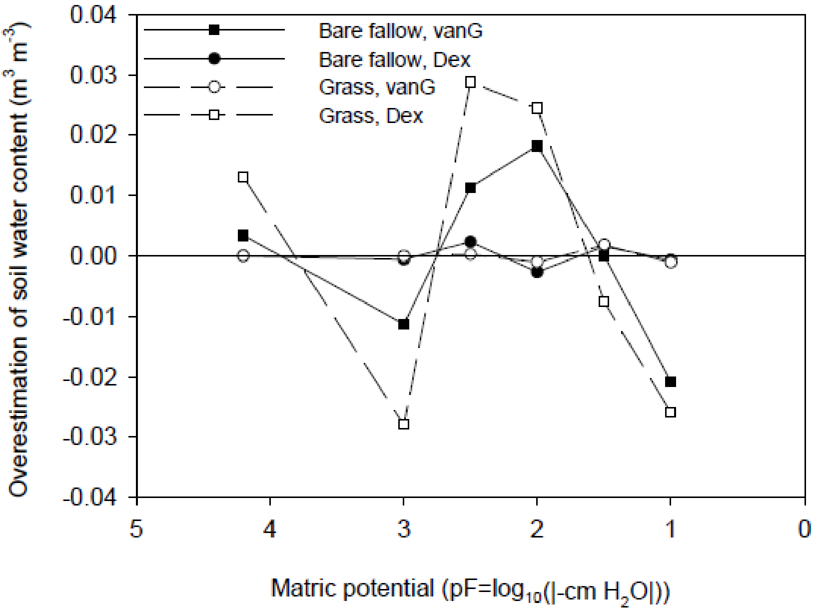

Fig. 7. Overestimation of soil water content (fitted-measured values) for the bare fallow (black symbols) and grass (white symbols) treatment at Highfield when fitted to the van Genuchten (vanG) model (square symbols) and the double-exponential (Dex) model (circle symbols) as a function of matric potential.

Introducing systematic errors depending on management (i.e. SOC and tillage) may have severe impacts when modelling key soil processes. We recommend using more flexible models such as the Dex model to describe the Q/I relation since it was better able to take into account the real variation in the distribution of pore sizes across the entire range of I. At the same time, we discourage uncritical use of uni-modal models such as the vanG model.

CONCLUSIONS

The bi-modal double-exponential (Dex) model provided a better fit to soil water retention data for relatively sandy Danish glacial till top- and subsoils, a silt loam and a sandy loam soil than the uni-modal van Genuchten (vanG) model. However, neither of the models worked well for highly sorted soils. Topsoil was less well described than subsoil when using the vanG model due to a more pronounced bi-modality of the size distribution of pores caused by increased SOC content and tillage. Similarly, RMSE of the vanG fit increased with an increase in SOC when going from the bare fallow to the grass treatment at Highfield. At the same time, the tillage intensity decreased, but for these long-term treatments, the effect of SOC seemed to outweigh the lack of tillage. These observations were reflected in a more pronounced bi-modality of the size distribution of pores for better structured soils. Consequently, we suggest that uni-modal models are too simplistic for describing management effects on PSD. Structural void ratio (V_2) estimated by the Dex model increased with SOC content for Highfield and with tillage intensity for Flakkebjerg, whereas the degree at which the soil is sorted (spread of particle sizes) was the primary driver affecting V_2 for Danish top- and subsoil samples.

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Figure captions

Fig. 1. The root mean squared error (RMSE) value for the Danish top- and subsoil of the Jakobsen data set using the van Genucthen (vanG) or double-exponential (Dex) model.

Fig. 2. (a) Measured volumetric water content for the four treatments at Highfield and fits of the double-exponential (Dex) model as a function of matric potential. The standard error of the mean are indicated (n=4). **(b)** Pore size distribution (d□/d(pF)) as a function of matric potential for the four treatments. Eq. 5 was used to obtain the pore size distributions.

Fig. 3. The root mean squared error (RMSE) value as a function of soil organic carbon (SOC) for the four treatments at Highfield using the van Genucthen (vanG) model (circle symbols) and the double-exponential (Dex) model (triangle symbols).

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