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Predicting soil particle density from clay and soil organic matter contents

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ABSTRACT

Soil particle density (Dp) is an important soil property for calculating soil porosity expressions. However, many studies assume a constant value, typically 2.65 Mg m^{-3} for arable, mineral soils. Few models exist for the prediction of Dp from soil organic matter (SOM) content. We hypothesized that better predictions may be obtained by including the soil clay content in least squares prediction equations. A calibration data set with 79 soil samples from 16 locations in Denmark, comprising both topsoil and subsoil horizons, was selected from the literature. Simple linear regression indicated that Dp of clay particles was approximately 2.86 Mg m^{-3}, while that of sand + silt particles could be estimated to ~2.65 Mg m^{-3}. Multiple linear regression showed that a combination of clay and SOM contents could explain nearly 92% of the variation in measured Dp. The clay and SOM prediction equation was validated against a combined data set with 227 soil samples representing A, B, and C horizons from temperate North America and Europe. The new prediction equation performed better than two SOM-based models from the literature. Validation of the new clay and SOM model using the 227 soil samples gave a root mean square error and mean error of 0.041 and +0.013 Mg m^{-3}, respectively. Predictions were accurate for all levels of SOM content in the validation data set. The model gave very precise predictions for soils with clay contents lower than 0.3 kg kg^{-1}, while a moderate over-prediction was observed for soils very high in clay. Finally, we developed a texture-enhanced curvilinear model that will be useful for predicting Dp of soils with high contents of clay and in particular SOM.

1. Introduction

Soil particle density (Dp) is an important soil property used in calculation of porosity and void ratio. Typically Dp is not measured but assumed a constant (e.g., Dp = 2.65 Mg m^{-3}). Void ratio is often used in soil mechanics (e.g., Keller et al., 2011), and reliable estimates are important in the interpretation of soil mechanical behavior. Similarly, models on soil aeration by diffusion and convection are based on the volume of air-filled pores (e.g., Schjønning et al., 2013), which also depends on accurate estimates of soil porosity. The lack of measured Dp in many soil studies may relate to the rather laborious measurement procedure (Blake and Hartge, 1986). However, a range of studies have documented that Dp actually varies considerably across soil types and geographical regions (e.g., Ball et al., 2000; Rühlmann et al., 2006).

Dp decreases with increasing content of soil organic matter (SOM), and prediction equations based on SOM content have been suggested (e.g., Bielders et al., 1990; Knott et al., 1987; McBride et al., 2011, 2012; Rühlmann et al., 2006). Rühlmann et al. (2006) found an effect of the mineral matrix, but did not include it in a model together with the effect of SOM. McBride et al. (2012) identified an effect of the content of clay (<0.002 mm) particles for a number of soils in North America. To our knowledge, however, no studies have yet combined the clay and SOM effects in prediction equations for Dp. Subsoils are generally very low in SOM content. Therefore, equations based solely on SOM content would give very similar predictions independent of soil texture. The objective of this study was to evaluate the potential in predicting soil Dp from the contents of clay particles and SOM. We hypothesized that the inclusion of clay as an additional determinant of Dp will increase the prediction strength of pedotransfer functions (PTFs) compared to existing models based solely on SOM. The investigation was based on an existing data set including a total of 79 soils. The PTF developed was tested on independent data from the literature and compared with two existing prediction equations based on only SOM content.

2. Materials and methods

2.1. Calibration data set

A study on soil hydraulic properties included a total of 79 soils originating from 16 Danish locations each with 4–5 soil horizons to a depth of 1 m. The results were published as a Departmental report (Jacobsen,

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1989) that can be downloaded from the internet. Clay and SOM contents of soils in the Jacobsen (1989) data set range from 0.015 to 0.375 and 0.000 to 0.062 kg kg^{-1}, respectively (Table 1). The large difference between the mean and the median value of SOM content indicates that most of the soils are subsoils. The soil parent materials include glacial deposits from the Weichsel glacial stage (10 soils) and the Saale glacial stage (one soil). Two soils were sampled in the raised Holocene sea floor and one in the present-day marine marsh area in southwestern Jutland. And finally, two soils represent Weichsel glaciofluvial deposits. The sand fraction is dominated by quartz, while the silt material is a combination of quartz, feldspars and other minerals (Møberg et al., 1988). The clay fraction is dominated by illite, typically increasing with depth. Kaolinite and smectite are present in varying degrees. Møberg et al. (1988) provides a thorough description of Danish soils. Jacobsen (1989) used the standard water pycnometer method for determination of Dp (Blake and Hartge, 1986).

2.2. Data sets for validation

Three studies were identified with tabulated values of soil particle-size distribution, SOM content and Dp. Hansen (1976) reported results from 50 Danish, arable soils including top- and subsoils. The ranges in clay content, SOM content and Dp were 0.016–0.276 kg kg^{-1}, 0.001–0.051 kg kg^{-1} and 2.51–2.76 Mg m^{-3}, respectively. Keller and Håkansson (2010) merged a range of Swedish data sets from agricultural field experiments comprising 123 topsoil samples. Clay content, SOM content and Dp ranged as follows: 0.045–0.697 kg kg^{-1}, 0.010–0.122 kg kg^{-1} and 2.39–2.69 Mg m^{-3}. Finally, Joosse and McBride (2003) reported data from 54 mineral soil horizons in 18 soil profiles at seven locations across temperate North America. These soils included different land use and A, B as well as C horizons (to a depth of 1.5 m), and the range in clay content, SOM content and Dp were 0.132–0.656 kg kg^{-1}, 0.000–0.228 kg kg^{-1} and 2.311–2.751 Mg m^{-3}, respectively. We note that the two latter data sets include soils with clay and SOM contents considerably higher than in the Jacobsen (1989) data set used for developing the PTF.

2.3. Existing models for particle density prediction

Two prediction equations for Dp were selected from the literature. Rühlmann et al. (2006) studied 170 soils from locations worldwide and from different soil layers. SOM content ranged from 0 up to nearly 100% expressed on a SOM plus mineral substance basis. They found that Dp could be estimated from SOM content by a curvilinear function as follows:

$$\mathrm{Dp} = \left[\frac{\mathrm{SOM_R}}{(\mathrm{a} + \mathrm{b} \times \mathrm{SOM_R})} + \frac{(1 + \mathrm{SOM_R})}{\mathrm{Dp_{min}}}\right]^{-1} \quad (1)$$

where $\mathrm{SOM_R}$ (kg kg^{-1} soil) is SOM given as a weight fraction relative to the sum of SOM and minerals. a and b are constants, 1.127 and 0.373, respectively, and $\mathrm{Dp_{min}} = 2.684$ Mg m^{-3} is the Rühlmann et al. (2006) estimate of Dp for SOM-free mineral substances.

McBride et al. (2011) collected a comprehensive data set including 282 soil horizons (A, B and C) from 91 profiles in southwestern Ontario, Canada. Their data covered a wide textural range and yielded the following prediction equation:

$$\mathrm{Dp} = 2.646–2.8 \times \mathrm{SOM} \quad (2)$$

Table 1
Key characteristics of the Jacobsen (1989) data set used for developing the PTF. SOM is soil organic matter content and Dp is particle density.

	Clay (<2 μm)	Silt (2–63 μm)	Sand (63–2000 μm)	SOM	Dp
	kg kg^{-1}				Mg m^{-3}
Mean	0.128	0.269	0.602	0.012	2.654
Median	0.121	0.275	0.580	0.005	2.657
Minimum	0.015	0.015	0.201	0.000	2.536
Maximum	0.375	0.672	0.965	0.062	2.716

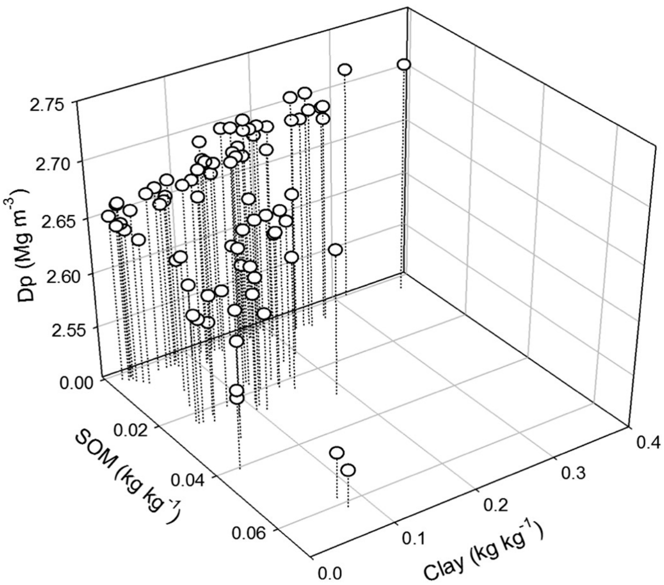

Fig. 1. Relation between particle density, Dp, and the contents of soil organic matter, SOM, and clay (particles <2 μm) for 79 Danish soils tabulated in the Jacobsen (1989) study.

2.4. Statistics

Multiple linear regression was used to identify how Dp related to SOM and clay contents of the Jacobsen (1989) data set (PROC REG; SAS Institute Inc., Cary, NC, USA). The Variance Inflation Factor (VIF) was calculated for the two predictors. VIF expresses the degree of multicollinearity among predictors in the regression. It provides an index that measures how much the variance of an estimated regression coefficient is increased because of collinearity. Upper value limits of VIF for non-erroneous conclusions from multiple regressions have been set at 5 (Menard, 1995; Rogerson, 2001) or 10 (Kutner et al., 2004).

The root mean square error (RMSE) and mean error (ME) were calculated to compare measured and predicted values:

$$\mathrm{RMSE} = \sqrt{\frac{1}{m}\sum_{i=1}^{m} d_i^2} \quad (3)$$

$$\mathrm{ME} = \frac{1}{m}\sum_{i=1}^{m} d_i \quad (4)$$

Table 2
Simple linear regression equations for selected statistically significant correlations. Root mean square error (RMSE) is in Mg m^{-3}. The numbers in parentheses are standard errors of estimate. P-values are valid for the model as well as for both coefficients (intercept and slope).

Equation	Eq. no.	r^2	RMSE	P > F
Full data set, n = 79				
Dp = 2.686(0.003) − 2.649(0.170) × SOM	(5)	0.769	0.019	<0.0001
Dp = 2.610(0.007) + 0.337(0.044) × Clay	(6)	0.433	0.030	<0.0001
Dp = 2.947(0.038) − 0.337(0.044) × [Sand + Silt]	(7)	0.433	0.030	<0.0001
Data with SOM < 0.01 kg kg^{-1}, n = 47				
Dp = 2.648(0.003) + 0.209(0.018) × Clay	(8)	0.766	0.010	<0.0001
Dp = 2.856(0.015) − 0.209(0.018) × [Sand + Silt]	(9)	0.766	0.010	<0.0001