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Carbon-sensitive pedotransfer functions for plant available water

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Abbreviations: NAPESHM, North American Project to Evaluate Soil Health Measurements; SOC, soil organic carbon; θ_{AWHC} , plant available water holding capacity; θ_{FC} , volumetric water content at field capacity; θ_{PWP} , volumetric water content at permanent wilting point.

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Abstract

Currently accepted pedotransfer functions show negligible effect of management-induced changes to soil organic carbon (SOC) on plant available water holding capacity (θ_{AWHC}), while some studies show the ability to substantially increase θ_{AWHC} through management. The Soil Health Institute's North America Project to Evaluate Soil Health Measurements measured water content at field capacity using intact soil cores across 124 long-term research sites that contained increases in SOC as a result of management treatments such as reduced tillage and cover cropping. Pedotransfer functions were created for volumetric water content at field capacity (θ_{FC}) and permanent wilting point (θ_{PWP}). New pedotransfer functions had predictions of θ_{AWHC} that were similarly accurate compared with Saxton and Rawls when tested on samples from the National Soil Characterization database. Further, the new pedotransfer functions showed substantial effects of soil calcareousness and SOC on θ_{AWHC} . For an increase in SOC of 10 g kg⁻¹ (1%) in noncalcareous soils, an average increase in θ_{AWHC} of 3.0 mm 100 mm⁻¹ soil (0.03 m³ m⁻³) on average across all soil texture classes was found. This SOC related increase in θ_{AWHC} is about double previous estimates. Calcareous soils had an increase in θ_{AWHC} of 1.2 mm 100 mm⁻¹ soil associated with a 10 g kg⁻¹ increase in SOC, across all soil texture classes. New equations can aid in quantifying benefits of soil management practices that increase SOC and can be used to model the effect of changes in management on drought resilience.

1 | INTRODUCTION

If plant available water holding capacity (θ_{AWHC}) increases in a meaningful way when soil organic carbon (SOC) increases, the outcome is that management practices that increase SOC in soils simultaneously change water retention by soils. This change in water retention has implications for hydrology, the energy balance, and crop production. Thus, a positive, causal, relationship between SOC and θ_{AWHC} has direct benefit through increased cropping system resilience to drought and provides an incentive for the adoption of practices that benefit society through climate change mitigation and adaptation (Lal, 2004; Lal, 2006; A. Williams et al., 2016; Yang et al., 2014). Soil science literature is inconclusive on whether this relationship exists to a meaningful degree in agricultural soils. Some studies have demonstrated substantial improvements in θ_{AWHC} as a result of increasing SOC (Ankenbaur & Loheide, 2017; Bouyoucos, 1939; Hudson, 1994; Maynard, 2000; Salter & Howarth, 1961) and others have not (Bauer & Black, 1992; Bell & Van Keulen, 1995; Feustal & Byers, 1936). A recent review concluded that the effect of SOC on θ_{AWHC} was limited; a 10 g kg⁻¹ increase in SOC concentration resulted in a θ_{AWHC} increase of 1.2 mm 100 mm⁻¹ soil (0.012 m³ m⁻³) across all soil textures (Minasny & McBratney, 2018). Meanwhile, those that promote management changes to improve soil health and functioning in agri-

cultural landscapes, such as drought resilience, are limited to providing regional and anecdotal evidence that increased SOC improves θ_{AWHC} .

While this debate is ongoing, researchers in disciplines like hydrology and land surface modeling, are relying on existing pedotransfer functions relating SOC to water characteristics. Pedotransfer functions allow practical estimation of field and laboratory soil measurements that are costly, time-consuming, and can be impractical to measure (Bouma, 1989) using proxy variables such as particle size, bulk density, and organic C to predict soil hydraulic properties of interest (Wösten et al., 2001). Soil scientists and engineers have a long history of estimating soil water characteristics that are difficult to measure (Brooks & Corey, 1964; Campell, 1974; Rawls et al., 1992; Van Genuchten, 1980) and early efforts demonstrated that soil particle size could predict soil water characteristics to provide adequate estimates for many decisions (Ahuja et al., 1985; Arya & Paris, 1981; Gupta & Larson, 1979; Saxton et al., 1986; J. Williams et al., 1983). Early pedotransfer functions were accurate, but many had limited geographic use because they were based on regional data (Gijssman et al., 2002).

Saxton and Rawls (2006) updated pedotransfer functions (Saxton, Rawls, Romberger & Papendick, 1986) for volumetric water content at field capacity (estimated by water retained at -33 kPa) and permanent wilting point (estimated by water

retained at $-1,500$ kPa). The difference between volumetric water content held at field capacity (θ_{FC}) and wilting point (θ_{PWP}) estimates θ_{AWHC} . The Saxton and Rawls (2006) pedotransfer functions were created with approximately 2,000 soil samples from A horizons obtained from the Natural Resource Conservation Service (NRCS) National Soil Characterization database (Soil Survey Staff, 2004). Saxton and Rawls (2006) did not report the depth of A horizon used, but the depth is likely well represented by the horizons in the National Cooperative Soil Survey Characterization (NCSS) Microsoft Access database, in which A master horizons were log normally distributed and ranged in depth from 0 to 60 cm with a median depth of 13 cm. The pedotransfer functions were fit using continuous sand, clay, and soil organic matter content and two-way interaction terms as predictor variables in a multiple linear regression. To improve the fit, a second nonlinear function was added resulting in two combined, dependent equations for prediction of θ_{FC} and θ_{PWP} .

The accuracy and continental distribution of the input data enabled these pedotransfer functions to be widely used (1,185 citations according to Scopus as of August 2021), while their simplicity resulted in their incorporation into many models. The high degree of use of these pedotransfer functions is illustrated by the number of agronomic, ecological, hydrological, land surface, and meteorological models listed in publications that cite Saxton and Rawls (2006) including the Soil Water Assessment Tool (SWAT), AquaCROP, Agricultural Policy/Environmental eXtender (APEX), Noah-MP land surface model, Soil-Plant-Air-Water (SPAW), Variable Infiltration Capacity (VIC), TOPMODEL, Agricultural Production System Simulator (APSIM), Annualized Agricultural Non-Point Source Pollution Model (AnnAGNPS), DeNitrification-DeComposition and DayCent. Because pedotransfer functions may be either hardcoded into models or used in the data preparation step to generate model input, this is not an exhaustive measure of the use of these functions.

Pedotransfer functions may be as simple as a look-up tables or as complex as machine learning techniques, including artificial neural networks and bootstrapping (Moosavi & Sepaskhah, 2012), support vector machines (Twarakavi et al., 2009), classification and regression trees (Pachepsky et al., 2006), and random forests and boosted regression trees (Jorda et al., 2015). Machine learning can provide more accurate predictions (Jorda et al., 2015) but their complexity means that the mathematical structure of the pedotransfer function is not easily published. Pedotransfer functions built using machine learning require software development to support them (Zhang & Schaap, 2017) and reduce the ease of implementing the function in larger computer models (Schaap et al., 2004). A comparison of 11 pedotransfer functions with varying levels of complexity for water retention found no superior model (Schaap, Nemes & van Genuchten, 2004), indicating that simple models can be adequate.

Core Ideas

- New pedotransfer functions show organic C increases plant available water.
- Noncalcareous soils show greater effects of organic C on plant available water.
- Increase in plant available water from organic C is more than double previous estimates.
- These pedotransfer functions can easily be used in hydrologic models.
- A gap is bridged for modeling the effect of increased soil organic C on plant available water.

Most existing pedotransfer functions include SOC (or soil organic matter), but the effects of SOC on θ_{AWHC} are reported as negligible (e.g., Saxton & Rawls, 2006; Minasny & McBratney, 2018). There is a mismatch between soil science textbooks and pedotransfer functions on the effects of SOC on θ_{AWHC} . For example, a textbook by Brady and Weil (2002) states that “Recognizing the beneficial effects of organic matter on plant available water is essential to wise soil management” indicating that SOC increases θ_{AWHC} to a meaningful degree in terms of crop production, yet pedotransfer functions do not give such results. This discrepancy could be explained by two nonmutually exclusive elements of the underlying data. First, θ_{FC} measurements may lack the effects of soil structure. This is particularly relevant for soil samples that are dried and sieved prior to θ_{FC} measurement. Disturbed soils may show the direct effect of SOC on water retention, but do not capture the secondary effects of SOC that manifest through soil structure because they do not contain interpedal pores. It is preferable to use intact soil clods or cores because they are more likely to capture both direct effect of SOC on water retention and the secondary effects of SOC that manifest through soil structure (Dane & Hopmans, 2018; J. Williams et al., 1983). Soil organic C has a strong link to soil structure (Bronick & Lal, 2005), and soil structure is linked to pore size distribution, which affects soil water at the macro scale (Nimmo & Akstin, 1988; Pachepsky & Rawls, 2003; J. Williams et al., 1983). Second, many datasets may include measurements of intact soil structures for building pedotransfer functions but were collected to represent changes between soil pedons (at the m scale) for the purpose of mapping and inventory. Hence when considering a given texture class, changes in SOC in such databases are not primarily influenced by management, but rather the landscape position and climate from which the soils were collected.

An additional consideration in creating pedotransfer functions for θ_{AWHC} is the effect of calcareousness. Calcareous soils have been reported to require more frequent irrigation

than noncalcareous soils to achieve the same crop yield, indicating that they may have lower θ_{AWHC} . Substantial amounts of calcium carbonate have been found to lower water retention in repacked soil samples (Stakman & Bishay, 1975) and to increase bulk density (Habel, 2014). It has been proposed that presence of calcium carbonate may alter water retention not only through changes in effective soil texture (e.g., carbonates the size of silicate clays), but also via alteration of soil structure and pores (Jackson & Eire, 1973), although analysis on intact samples would be needed to confirm such an effect. We found, in this data set, a significant effect of calcium carbonate on predictions of θ_{AWHC} .

The Soil Health Institute's North America Project to Evaluate Soil Health Measurements (NAPESHM) provided a unique dataset to investigate whether increases in SOC as a result of management correspond to increases in θ_{AWHC} . The NAPESHM dataset contains a broad distribution of agricultural soils, primarily managed for row crops, across the major cropland regions of United States, Canada, and Mexico. Data were collected on replicated experimental units (either plots or fields that represent one replication of a treatment) under long-term treatments (10 yr or more) within research sites ($n = 124$). This approach is expected to capture variation in SOC and measured θ_{AWHC} that are both management induced (within pedons) and inherent (between pedons). Additionally, θ_{FC} (estimated by water retained at -33 kPa) was measured on intact cores, thus capturing the effect of SOC on the soil matrix and bulk soil (including soil structure).

The goal of this work was to create a simple-to-implement pedotransfer function for θ_{AWHC} that is sensitive to changes in SOC. To meet our goal, we used simple linear regression to fit functions for θ_{FC} and θ_{PWP} using NAPESHM data. We assessed the accuracy of predicted θ_{FC} , θ_{PWP} , and θ_{AWHC} (by subtraction of predicted θ_{FC} and θ_{PWP}) to the accuracy of Saxton and Rawls (2006) on 1,797 soils from NCSS. The Saxton and Rawls (2006) approach was chosen as a comparison because of its ubiquity in hydrology and energy models, its representation of similar geographical extent, and its similar simplicity of modeling approach. We also considered how four levels of SOC affected predictions made by the new pedotransfer functions and compared these results to Saxton and Rawls (2006) pedotransfer functions and literature.

2 | MATERIALS AND METHODS

Data used to develop new pedotransfer functions were drawn from the NAPESHM database, which captured a range in climate, management practices, and inherent soil properties using 124 long-term agricultural research sites across North America and were uniformly sampled in 2019 (Norris et al., 2020). Soil orders in the dataset included the Soil Taxonomy orders of Ultisol, Alfisol, Mollisol, Vertisol, Aridisol,

Inceptisol, and Entisol. The replicated treatments included tillage, residue management, cover crop use and type, crop rotation, grazing, and nutrient type and rate (including organic amendments). At the time of sampling, most treatments in the NAPESHM database were continuous for 10 or more years.

To develop new pedotransfer functions, we used measurements of particle size distribution, SOC, inorganic C, bulk density, and gravimetric water content measured at field capacity (-33 kPa) and permanent wilting point ($-1,500$ kPa). Soil particle size analysis, pH, and SOC were measured at The Ohio State Soil Water and Environmental Lab. Bulk density and all measures of water retention were done at the Cornell Soil Health Laboratory (Ithaca, NY). Particle size distribution, SOC, and θ_{PWP} were measured using a composite soil sample collected from 0-to-15-cm depth from four to six sampling locations within each experimental unit (Norris et al., 2020). The sieve and pipette method with three size classes (2,000–50, 50–2, and <2 μm) was used to measure soil particle size distribution (Gee & Bauder, 1986). Total C was measured by dry combustion (Nelson & Sommers, 1996) using an NC 2100 soil analyzer made by CE instruments (Lakewood, NJ). Soils were oven dried and ground. Soils with >7.2 pH (1:2, soil/water) (Thomas, 1996) were tested for effervescence with 10% HCl. Those that effervesced were analyzed for carbonates using the Chittick's volumetric calcimeter method (Dreimanis, 1962). For soils with carbonates, SOC was calculated by subtracting the value of inorganic C from total C obtained by dry combustion. For all other samples, total C obtained using dry combustion represented SOC.

In addition to the composite soil sample, four 7.6-cm diam. soil cores were collected to a depth of 7.6 cm in each experimental unit and maintained intact using a plastic sleeve. Two of the four cores were kept intact for measuring bulk density and θ_{FC} . The remaining two cores were composited into one bag, sieved to remove coarse fragments >2 mm, and used to calculate soil bulk density. For any sample with $<2\%$ coarse fragments by weight (determined during preparation for particle size analysis), bulk density was calculated as the mean bulk density of all four cores—two intact and two composited. Ninety percent of the experimental units in this study had $<2\%$ coarse fragments by weight. For the remaining 10% with coarse fragments $>2\%$ by weight, bulk density was calculated as the mean of the two composited cores, following removal of coarse fragments and adjustments for the weight and volume of coarse fragments.

Gravimetric water content at permanent wilting point was measured on pressure plates at 1,500 kPa (Reynolds & Topp, 2008) using repacked soil from the composite sample. Each sample used 15 g of soil that was dried (105 $^{\circ}\text{C}$), ground (2-mm sieve), saturated, repacked, and equilibrated for 7 d on the pressure plate at 1,500 kPa. Two replications were measured per experimental unit and the mean was calculated to represent θ_{PWP} for each experimental unit. Gravimetric water

content at field capacity was measured on both intact cores using a tension table at 33 kPa (Hao et al., 2008; Topp et al., 1993). The mean of the two intact cores represented the θ_{FC} for each experimental unit. For the intact cores used to calculate θ_{FC} , the cores were first saturated (4–7 d), equilibration times on the tension table were between 4 and 7 d, and reference samples were used (weight recorded daily) for quality control. Both θ_{FC} and θ_{PWP} were calculated by multiplying gravimetric water content by the mean bulk density of the experimental unit and assuming a density of water of 1.0 Mg m^{-3} . Plant available water-holding capacity was calculated as the difference between θ_{FC} and θ_{PWP} .

We removed extreme values from our analysis. Experimental units that were excluded were those with a mean bulk density $>1.8 \text{ Mg m}^{-3}$ and SOC concentrations $>46.5 \text{ g kg}^{-1}$. No samples had mean bulk density of $<1.0 \text{ Mg m}^{-3}$. Our threshold values for bulk density and SOC were the same as those used to develop the Saxton and Rawls (2006) pedotransfer functions. The final NAPESHM dataset used in this study included 1,731 samples for development of pedotransfer functions. These 1,731 samples represented 547 unique management treatments across 119 sites. Most sites (107) had been managed continuously for 10 or more years, although 12 sites had at least one treatment that had been in place for between 5 and 10 yr. Figure 1 shows the distribution of site locations across North America, with Hargreaves' moisture deficit, to demonstrate the range in climatic conditions. Eleven of the 12 USDA soil texture classes were represented in the NAPESHM data used in this study (Table 1); sandy clay textures were not represented. The most abundant texture classes were silt loam and loam. Soils were predominantly sampled in the United States, with 1,335 experimental units from 91 sites. Fifteen sites (237 experimental units) were in Canada, and 13 sites (161 experimental units) were in Mexico. Soil organic C ranged from 2 to 44 g kg^{-1} with a median of 14 g kg^{-1} . In total, 335 samples from 35 sites effervesced when treated with 10% HCl. Few calcareous soils had relatively high SOC; there were 63 experimental units with $>20 \text{ g kg}^{-1}$ SOC, including 12 $>30 \text{ g kg}^{-1}$ SOC, and 3 $>40 \text{ g kg}^{-1}$ SOC (Figure 2a). For noncalcareous soils, there were 322, 32, and 2 experimental units that were >20 , 30, and 40 g kg^{-1} SOC, respectively. Most of the noncalcareous soils with greater SOC were between 10 and 40% clay content (Figure 2a) and two experimental units were $>30 \text{ g kg}^{-1}$ SOC and more than 40% clay. Calcareous soils were well distributed across the observed clay contents and largely followed the same trends as noncalcareous soils when θ_{FC} and θ_{PWP} were plotted against clay content (Figure 2b,c). There was greater variance in water content for θ_{FC} than for θ_{PWP} , which is consistent with theory and practice (Pachepsky & Rawls, 2003; Saxton & Rawls, 2006).

Hargreaves' moisture deficit used for the map in this study was generated with the ClimateNAv5.10 software package

(available at <http://tinyurl.com/ClimateNA>) based on methodology described by Wang et al. (2016). Hargreaves' moisture index has a value of zero for any month within a year that has greater precipitation than reference evapotranspiration. For all months in which the precipitation is less than reference evapotranspiration, the difference is summed to arrive at the annual moisture deficit (mm).

To test the accuracy of the new pedotransfer functions, we obtained data from 1,797 soils from the National Cooperative Soil Survey Characterization (NCSS) database (<http://ncsslabsdatamart.sc.egov.usda.gov/>; Soil Survey Staff, 1995). These data included sampling locations from 39 U.S. states. All 12 USDA soil texture classes were represented in the noncalcareous soils and 10 classes were represented within calcareous soils. Each horizon started at 0 cm and ended at or before 15-cm depth and had measurements of bulk density (volume measured at -33 kPa), gravimetric water content at both permanent wilting point ($-1,500 \text{ kPa}$) and field capacity (at -33 kPa ; clod method; Soil Survey Staff, 2014), and total C, calcium carbonate, sand, and clay content. We multiplied gravimetric water content by bulk density to obtain θ_{FC} and θ_{PWP} . Soil organic C was calculated by subtracting the quantity of inorganic C in carbonates from total C. The NCSS data were developed with standard laboratory procedures (Klute, 1986; USDA-SCS, 1982).

We developed pedotransfer functions by initially fitting multiple linear regression models to the NAPESHM data using ordinary least squares for θ_{FC} and θ_{PWP} using clay, sand, SOC content (all units are in 10 g kg^{-1} , which is equivalent to 1.0%), and all two-way interaction terms as predictor variables. To determine whether there was a significant difference in the predictions of the pedotransfer functions for soils that were and were not calcareous, we conducted a one-way ANOVA on the regression residuals using a categorical indicator for effervescence when treated with HCl as the only factor. For all statistical analyses, R statistical software (R Development Core Team, 2020) and $\alpha = .001$ were used.

The ANOVA p value for the effect of calcareousness on water content was significant for model predictions of θ_{FC} ($p = .03$) but not for θ_{PWP} ($p = .45$). We fit separate models for calcareous soils (those that effervesced when treated with HCl) and noncalcareous soils. We then used backwards stepwise selection for each model by applying the step function from the stats package in R (Hastie & Pregibon, 1992). For both calcareous and noncalcareous soils, stepwise selection for θ_{FC} models showed the lowest AIC for the full models (clay, sand, SOC content, and all two-way interaction terms). For calcareous soils, the θ_{PWP} model that had the lowest AIC included clay, sand, and SOC content, and the two-way interaction terms for both SOC by sand content and SOC by clay content. For calcareous soils, stepwise selection for the θ_{PWP} model found that the lowest AIC resulted from clay, sand, and SOC content, and the two-way interaction term between sand

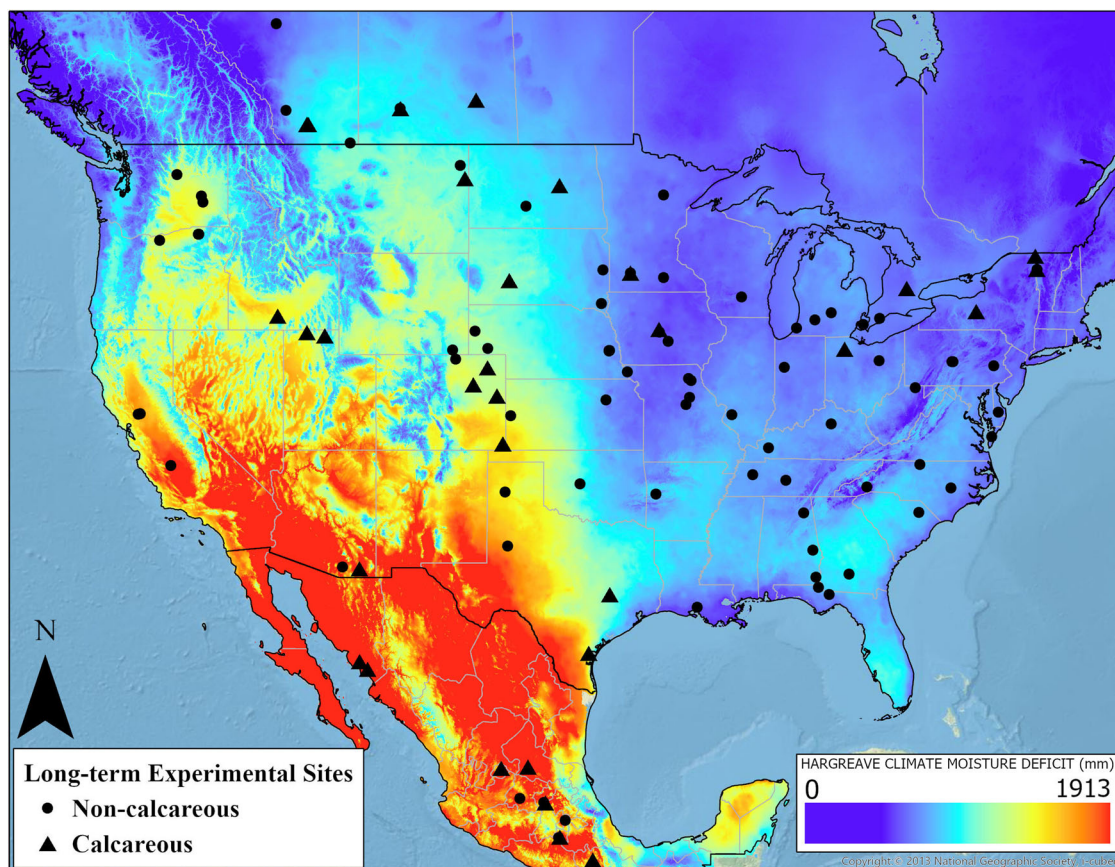


FIGURE 1 Soils were sampled at 124 sites for the North American Project to Evaluate Soil Health Measurements. The map shows Hargreaves' climate moisture deficit for the 119 sites used in this study

and clay content. For each linear model, plots of model residuals against model-fitted values and predictors were used to verify equal error variance and the Breusch–Pagan test against heteroskedasticity was also used. Plots of residuals vs. leverage (Cook's distance cutoff of 0.5) were used to check for influential values, and theoretical quantile-quantile plots were used to check normality of the residuals.

To investigate whether θ_{FC} and θ_{PWP} were responding to effects of soil management that were not manifested in SOC changes, we plotted model residuals against aggregate stability measured with a Cornell rainfall simulator, the average Soil Tillage Intensity Rating (STIR, Karlen et al., 2008; U.S. Department of Agriculture, 2019) calculated for the past 5 yr, and categorical variables designating crop category (row crop, perennial, integrated row crop and perennial, non-farmed, or woody perennial) and nutrient type (none, organic, synthetic, or synthetic and organic). We tested the strength of the relationship between model residuals and these variables (aggregate stability, STIR, crop category, nutrient type) using regression for continuous variables and ANOVA for categorical variables and found they did not explain substantial variance as shown by an R^2 of .03 or less for each regression or ANOVA. We reported the root mean square error (RMSE) and

adjusted R^2 from regressions of predictions on measurements for θ_{FC} , θ_{PWP} , and θ_{AWHC}

We predicted θ_{FC} and θ_{PWP} for 1,797 soils from the NCSS database using both the new pedotransfer functions and Saxton and Rawls (2006). We computed the deviation from measured values (predicted-measured) and RMSE for θ_{FC} , θ_{PWP} , and θ_{AWHC} (θ_{AWHC} calculated by subtraction) for both pedotransfer function predictions by USDA particle size class. We used a paired t test to determine significant differences from measured water content for both pedotransfer functions. Saxton and Rawls (2006) pedotransfer functions include an organic matter parameter, but we used a SOC parameter. Because the van Bemmelen factor (0.58) was used to convert SOC to organic matter to develop the Saxton and Rawls (2006) functions, we converted NCSS SOC values to organic matter by multiplying SOC by the reciprocal of the van Bemmelen factor.

To investigate the effect of SOC on predicted θ_{AWHC} , we generated values that represent possible combinations of SOC, clay, and sand content. These combinations of possible SOC, clay, and sand content values were not measured soil samples – rather they were created to evaluate a wide range of sand, clay, and SOC content. Soil organic C values of 10, 20,

TABLE 1 Count of experimental units ($n = 1,731$) and sites ($n = 119$) by USDA soil texture class. A single site may have multiple soil texture classes, so the sum of sites shown is greater than the number of sites in the study. Data shown is from North American Project to Evaluate Soil Health Measurements

USDA soil texture class	Sites	Experimental units
Noncalcareous		
Clay	7	17
Clay loam	20	148
Loam	34	265
Loamy sand	14	96
Sand	5	31
Sandy loam	26	193
Sandy clay loam	10	46
Silt	5	10
Silt loam	40	480
Silty clay	4	9
Silty clay loam	14	85
Calcareous		
Clay	6	60
Clay loam	12	25
Loam	18	112
Sandy loam	4	20
Sandy clay loam	1	2
Silt loam	6	23
Silty clay	6	63

30, and 40 g kg⁻¹ (1, 2, 3, and 4%) and clay and sand values from 5 to 95% in 5% increments were used and repeated so that each sand content was paired with every clay content and every level of SOC; resulting in 760 combinations in all. We used these combinations of SOC, clay, and sand content to generate predictions of θ_{FC} and θ_{PWP} using the new pedotransfer functions (both noncalcareous and calcareous) and Saxton and Rawls (2006) pedotransfer functions. Locally estimated scatterplot smoothing (LOESS) curves were fit to the predictions for each level of SOC for visual evaluation.

3 | RESULTS AND DISCUSSION

The pedotransfer functions for volumetric water content at θ_{PWP} and θ_{FC} are given in Equations 1 and 2 for noncalcareous soils and in Equations 3 and 4 for calcareous, respectively. All units are in 10 g kg⁻¹.

$$\theta_{PWP} = 7.222 + 0.296\text{Clay} - 0.074\text{Sand} - \underline{0.309\text{SOC}} + 0.022 (\text{Sand} \times \text{SOC}) + 0.022 (\text{Clay} \times \text{SOC}) \quad (1)$$

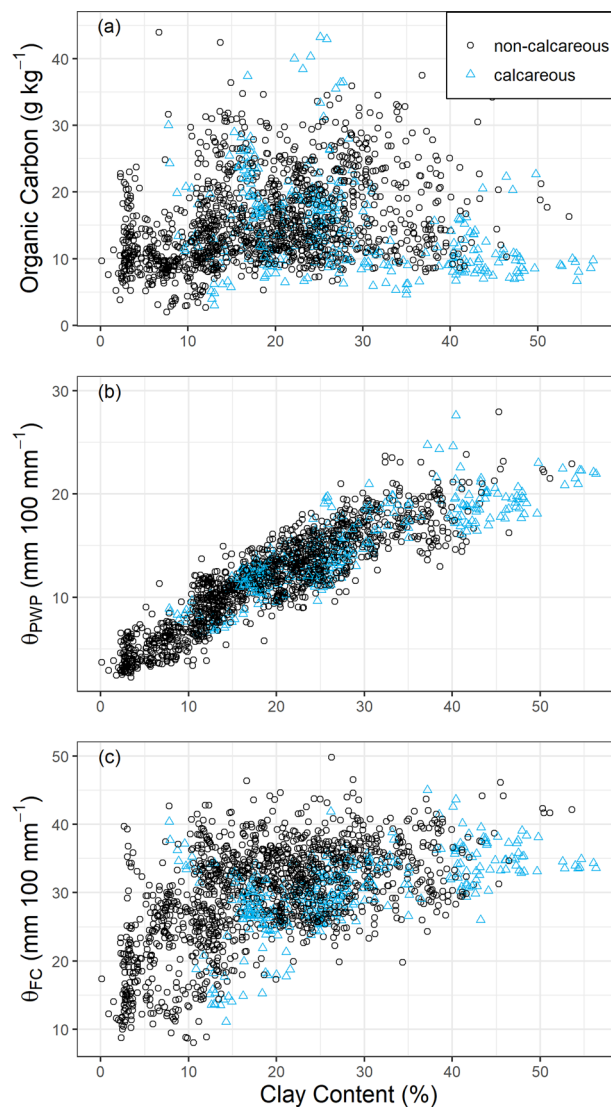


FIGURE 2 Organic C (%) and volumetric water content for permanent wilting point (θ_{PWP}) and field capacity (θ_{FC}), plotted against clay content. Data shown is from North American Project to Evaluate Soil Health Measurements

$$\theta_{FC} = 37.217 - 0.140\text{Clay} - 0.304\text{Sand} - \underline{0.222\text{SOC}} + 0.051 (\text{Sand} \times \text{SOC}) + 0.085 (\text{Clay} \times \text{SOC}) + 0.002 (\text{Clay} \times \text{Sand}) \quad (2)$$

$$\theta_{PWP,calc} = 7.907 + 0.236\text{Clay} - 0.082\text{Sand} + 0.441\text{SOC} + 0.002 (\text{Clay} \times \text{Sand}) \quad (3)$$

$$\theta_{FC,calc} = 33.351 + \underline{0.020\text{Clay}} - 0.446\text{Sand} + \underline{1.398\text{SOC}} + 0.052 (\text{Sand} \times \text{SOC}) - 0.077 (\text{Clay} \times \text{SOC}) + 0.011 (\text{Clay} \times \text{Sand}) \quad (4)$$

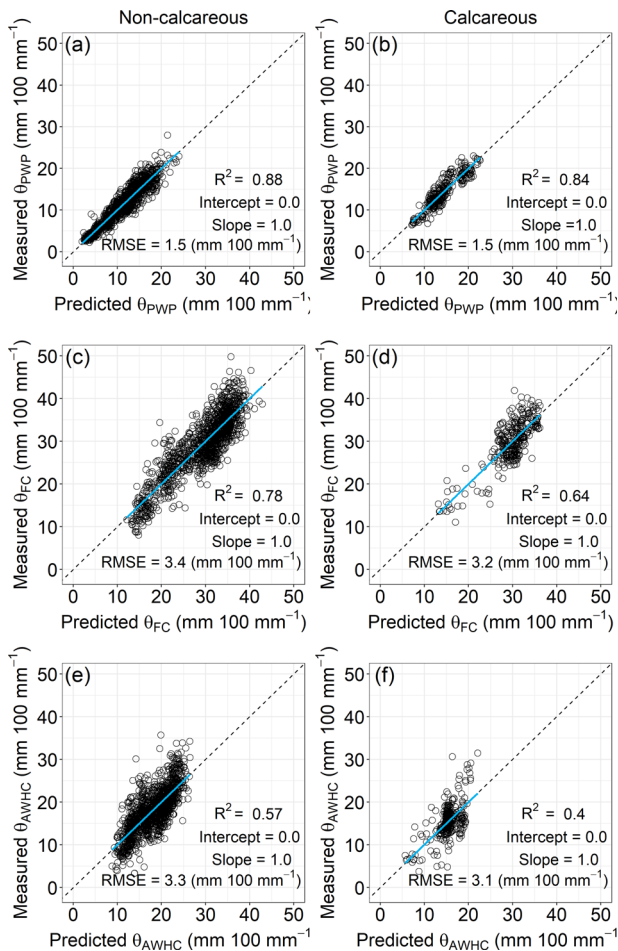


FIGURE 3 (a and b) Measured vs. predicted volumetric water content at permanent wilting point (θ_{pWP}) (c and d) field capacity (θ_{FC}), and (e and f) plant available water holding capacity (θ_{AWHC}) for (left) noncalcareous and (right) calcareous soils. Measured values are from the from North American Project to Evaluate Soil Health Measurements and predicted values are from new pedotransfer functions. Predictions of θ_{AWHC} are calculated by subtraction of predicted θ_{FC} and θ_{pWP} . Regressions are significant (p value < .001). Blue, solid lines are regression fits and black, dashed lines are one-to-one. RMSE is root mean square error

All terms were significant or were nonsignificant main effects that were retained as a component of a significant two-way interaction. The nonsignificant main effect coefficients are underlined in the equations above.

3.1 | Accuracy of new pedotransfer functions

We used regressions between pedotransfer function predictions and the measured NAPESHM data that was used to create the models as one test of accuracy (Figure 3). Models for predicting θ_{pWP} had better accuracy than for θ_{FC} , indicated by R^2 and RMSE. The models for noncalcareous soils performed better than models for calcareous soils. The new pedotransfer

functions are near the lower end of RMSE values for water retention predictions reported by Schaap et al. (2004), who found that of the 11 modes they considered, mean RMSE was between 3.2 and 6.9 mm 100 mm⁻¹. The error was slightly greater for θ_{AWHC} , ranging from 5.8 to 8.0 mm 100 mm⁻¹. Model performance of the Saxton and Rawls (2006) equations were also similar with R^2 and RMSE of 0.86 and 2.0 mm 100 mm⁻¹ for θ_{pWP} and 0.63 and 5.0 mm 100 mm⁻¹ for θ_{FC} , respectively. The lesser accuracy of the models for calcareous soils is likely from two sources. One being fewer experimental units used in the fit; the calcareous fit had 335, while the noncalcareous model had 1,396, and about 2,000 were used in Saxton and Rawls (2006). Secondly, the physical complexity of calcareous soils could also add to the poorer fit.

As a further test of accuracy and to provide context to evaluate the new pedotransfer functions, the new pedotransfer functions and Saxton and Rawls (2006) were used to calculate predictions of θ_{pWP} , θ_{FC} , and θ_{AWHC} (by subtraction of predicted θ_{FC} and θ_{pWP}) for 1,797 soils from the National NCSS database. Because the Saxton and Rawls (2006) pedotransfer functions were developed using NCSS data including θ_{FC} , it was expected that they would be more accurate in this test compared with the new pedotransfer functions using NAPESHM data including θ_{FC} . However, in general, new pedotransfer functions for noncalcareous soils performed similarly to Saxton and Rawls (2006) in regard to their RMSE (Table 2), although there were differences between particle size classes. Specifically, the new pedotransfer functions for noncalcareous soils had smaller RMSE values than Saxton and Rawls (2006) functions for θ_{pWP} , θ_{FC} , and θ_{AWHC} for coarse texture classes (sand, loamy sand, sandy loam, and silt loam). Saxton and Rawls (2006) functions had smaller RMSE values for θ_{pWP} , θ_{FC} , and θ_{AWHC} in finer textures (silty clay loam, sandy clay loam, clay loam, and all clays). For loams, the new pedotransfer functions had smaller RMSE values compared with Saxton and Rawls (2006) for θ_{FC} and θ_{AWHC} , but not for θ_{pWP} , while in silts, the reverse was true (Table 2). The greatest difference in RMSE magnitude for θ_{AWHC} of noncalcareous soils occurred in clay where the RMSE of the new pedotransfer functions was 3.3 mm 100 mm⁻¹ greater than the Saxton and Rawls (2006) pedotransfer functions (Table 2). In calcareous soils, unlike noncalcareous soils, RMSE values for the new pedotransfer functions were greater in coarser textures; sand had an RMSE for θ_{AWHC} that was 7.4 mm 100 mm⁻¹ greater compared with Saxton and Rawls (2006) but both pedotransfer functions had a relatively large RMSE for sand.

Deviations from measured NCSS data for both Saxton and Rawls (2006) and new pedotransfer function predictions are shown in Figure 4, and asterisks indicate that paired t tests found significant differences between predicted and measured water content ($\alpha = .001$). In noncalcareous soils, the new pedotransfer function predictions were significantly different

TABLE 2 Root mean square error (RMSE) values for volumetric water content at permanent wilting point (θ_{PWP}), field capacity (θ_{FC}), and plant available water holding capacity (θ_{AWHC}) predicted using both Saxton and Rawls (2006) (S&R) and the new pedotransfer functions using 1,797 soil samples from the National Cooperative Soil Survey Characterization database. The RMSEs are grouped by USDA soil texture classes and the number of samples (n) are shown for each texture class

USDA soil texture class	n	θ_{PWP}		θ_{FC}		θ_{AWH}	
		RMSE (mm 100 mm ⁻¹)					
		S&R	New	S&R	New	S&R	New
Noncalcareous							
Sand	39	3.4	2.3	10.2	7.8	7.9	6.9
Loamy sand	45	3.9	2.7	10.6	6.0	7.3	5.0
Sandy loam	169	7.3	6.5	13.6	9.0	8.3	5.8
Silt loam	273	4.9	4.0	8.9	6.0	6.3	5.4
Silt	4	3.6	2.1	5.6	6.1	5.4	6.6
Loam	198	4.5	4.9	9.6	7.3	7.0	5.2
Silty clay loam	201	2.8	4.7	4.2	5.2	4.7	4.8
Sandy clay loam	39	4.1	6.8	6.9	9.5	5.3	5.5
Clay loam	87	4.0	7.0	5.7	9.6	4.9	5.6
Silty clay	71	4.3	8.0	5.5	10.9	7.0	7.5
Sandy clay	10	3.1	8.4	4.8	13.6	4.9	7.0
Clay	113	5.2	8.1	5.1	14.0	5.1	8.4
Calcareous							
Sand	5	3.0	2.1	18.3	25.7	17.1	24.5
Loamy sand	12	5.3	4.7	12.6	15.9	8.5	12.4
Sandy loam	88	3.4	3.2	9.7	11.0	8.5	10.2
Silt loam	77	7.8	6.3	11.6	10.0	10.4	10.6
Loam	88	5.1	4.8	10.9	10.7	12.8	12.9
Silty clay loam	62	4.8	5.5	6.4	5.8	4.8	4.9
Sandy clay loam	51	2.9	3.2	4.4	4.3	3.4	3.6
Clay loam	55	7.0	6.0	4.3	5.3	8.7	8.3
Silty clay	34	5.6	6.8	6.6	6.8	3.9	3.9
Clay	75	10.1	7.6	5.8	9.2	9.7	9.4

from θ_{PWP} measurements in 11 texture classes, and Saxton and Rawls (2006) predictions were different for eight texture classes (Figure 4a). In calcareous soils, both the new pedotransfer function predictions and Saxton and Rawls (2006) were significantly different from θ_{PWP} measurements in four texture classes (Figure 4b). For θ_{FC} , and in noncalcareous soils, the new pedotransfer function predictions were significantly different from measurement in nine texture classes and Saxton and Rawls (2006) were significantly different in eight (Figure 4c). For calcareous soils, the new pedotransfer functions were significantly different from measured θ_{FC} in six texture classes and five for Saxton and Rawls (2006) (Figure 4d). For the new pedotransfer functions, deviations

from NCSS measurements in θ_{FC} and θ_{PWP} had bias in the same direction, and the bias was lost in subtraction when calculating θ_{AWHC} . This resulted in improved performance for θ_{AWHC} (Figure 4e,f). The new pedotransfer functions predictions for noncalcareous soil were different from measurements in clay and silty clay loam textures, while Saxton and Rawls (2006) predictions were different from measurements in six texture classes (Figure 4e). For calcareous soils, both pedotransfer functions were similarly different from NCSS measurements in four to five texture classes (Figure 4f). For θ_{AWHC} predictions, there was only one soil texture in which new pedotransfer function predictions were different from NCSS measurements. For noncalcareous soils, the difference occurred in clay and in loamy sand for calcareous soil.

For noncalcareous soils, the largest mean deviation from measured θ_{AWHC} was from Saxton and Rawls (2006) predictions in sandy loams and was 5.9 mm 100 mm⁻¹ (Figure 4e). For calcareous soils, the largest mean deviation from measured θ_{AWHC} was from the new pedotransfer function in sand and was 19.8 mm 100 mm⁻¹ (Figure 4f). Sand was under-represented in the model and the next highest mean deviation (loamy sand) was half as large at 10.8 mm 100 mm⁻¹. The comparison to NCSS data points out the new pedotransfer functions provided less accurate predictions of θ_{PWP} and θ_{FC} than Saxton and Rawls (2006), but predictions of θ_{AWHC} that were as or more accurate. The accuracy of the new pedotransfer functions is notable and encouraging, given that Saxton and Rawls (2006) functions were trained on NCSS data all using the same laboratory methodology for measurement (the clod method).

3.2 | Effect of soil organic C on predicted θ_{AWHC}

The point of presenting the new set of pedotransfer functions is their greater response to increases in SOC relative to existing equations. The overlapping of all four gold LOESS fits in Figure 5a through 5f demonstrate that while organic matter content is statistically significant in Saxton and Rawls (2006) pedotransfer function there is little discernable change in θ_{PWP} , θ_{FC} , and θ_{AWHC} as SOC varies (<0.074% volumetric water content in response to an increase from 1 to 4% SOC content). Conversely, the new pedotransfer functions show changes in θ_{PWP} , θ_{FC} , and θ_{AWHC} with discernable changes in SOC values. The LOESS curves fit to predictions of water content show that changes in response to SOC were greatest at θ_{FC} and least for θ_{PWP} (Figure 5). Earlier knowledge described uniform effect of SOC on water retention (Jong, 1983; Riley, 1981); however, our results agree with later findings by Minasny & McBratney (2018) that changes in water retention respond to SOC more for field capacity than for permanent wilting point. This effect of SOC was more pro-

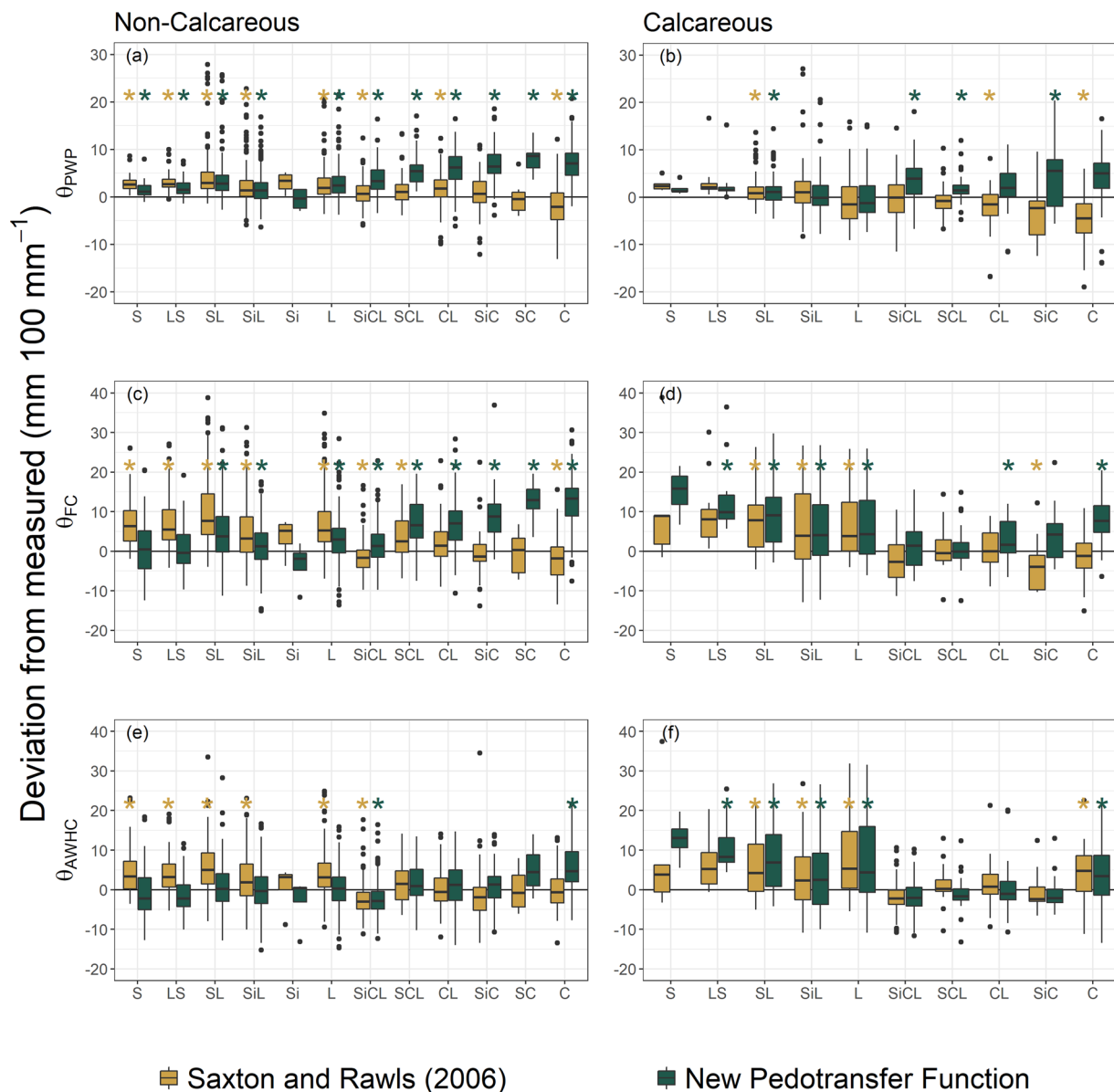


FIGURE 4 Deviation from measured (measured minus predicted) water contents. Measured data is from soil samples from the National Cooperative Soil Survey Characterization database for permanent wilting point (θ_{PWP}), field capacity (θ_{FC}), and plant available water holding capacity (θ_{AWHC}). Predicted values were generated with Saxton and Rawls (2006) and the new pedotransfer functions

nounced for noncalcareous soils. Importantly, the effect of SOC on water retention was consistent across for all levels of SOC, that is, a 10 g kg^{-1} increase in SOC produced the same increase in volumetric water content regardless of the initial SOC content (Figure 5).

For noncalcareous soils with clay content not represented in the NAPESHM dataset ($>60\%$) and SOC $<20 \text{ g kg}^{-1}$, the new pedotransfer functions predicted negative changes θ_{AWHC} values resulting from increased SOC. At these high clay contents, greater SOC causes θ_{PWP} to increase at a greater rate than θ_{FC} . This phenomenon was not expected, though similar outcomes have been reported in pedotransfer functions for saturated hydraulic conductivity (K_s). For example,

Nemes et al. (2005) found negative correlations between K_s and organic matter increases in several pedotransfer functions and the range of soils that exhibited this negative correlation was dataset dependent. The pedotransfer function may be improved by adding observations representing these greater clay contents. At present, we recommend restricting clay contents to 60% when using Equations 1 and 2, which is the same range of clay content for the dataset used to create Saxton and Rawls (2006) as well as other datasets, for example, UNSODA (Nemes et al., 2001).

Increases in SOC for calcareous soils with $>35\%$ clay content are also not represented well in the new pedotransfer functions, and there were only four calcareous experimental

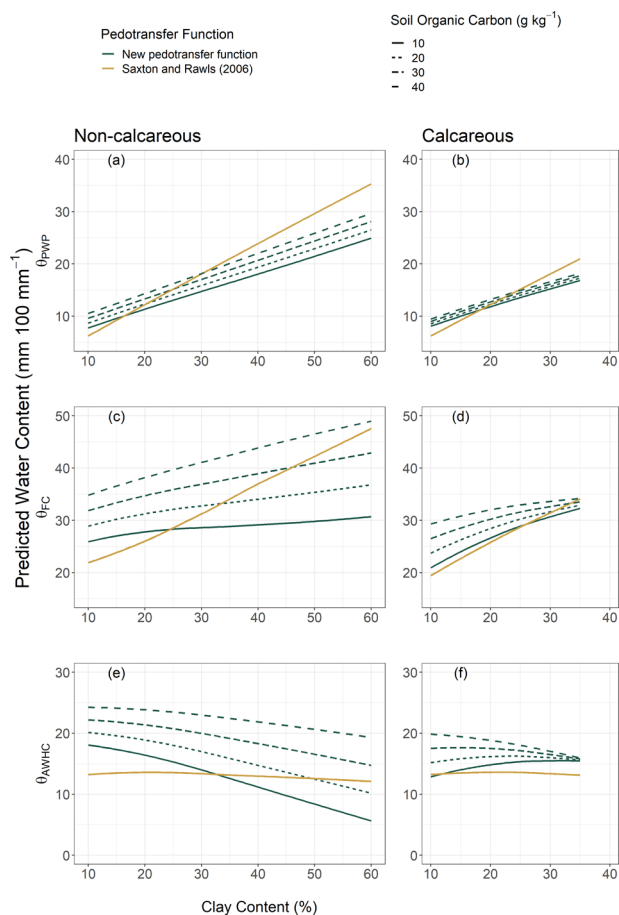


FIGURE 5 LOESS fits to predicted volumetric water contents for permanent wilting point (θ_{PWP}), field capacity (θ_{FC}), and plant available water holding capacity (θ_{AWHC}) using simulated data for both new and Saxton and Rawls (2006) pedotransfer functions. Lines for Saxton and Rawls (2006) pedotransfer functions at the four levels of soil organic C overlap

units that had 20 g kg^{-1} SOC or more. Because of this, we conclude that the usefulness of the calcareous functions are to illustrate that calcareous soils have different relationships with water holding capacity than noncalcareous soils. This difference is not well discussed in the soil science literature and needs more development. The new pedotransfer functions for calcareous soils (Equations 3 and 4) is not useful in soils with $>35\%$ clay, and we have limited Figure 3e and f accordingly.

It is notable that Saxton and Rawls (2006) pedotransfer functions have similar predictions to the new pedotransfer functions in situations of high and low clay content and correspondingly low and high SOC. For example, the LOESS curves fit to predictions in Figure 5c are all similar for 10 g kg^{-1} SOC at 10% clay content and 40 g kg^{-1} SOC at 60% clay content. We speculate that this is because SOC (and its effects on θ_{AWHC}) in the NCSS data used to fit Saxton and Rawls (2006) is not management induced. Rather, it is driven largely by inherent properties so that, in essence, the effects of SOC are indistinguishable from the effects of clay content. For

this reason, Saxton and Rawls (2006) pedotransfer functions are not able to capture the effects of improved soil management on θ_{PWP} , θ_{FC} , and θ_{AWHC} .

To quantify the effect of SOC on the new predictions, we calculated summary statistics for predictions of θ_{PWP} , θ_{FC} , and θ_{AWHC} using the same simulated soil samples to which we fit LOESS curves. The summary statistics demonstrate that effects of SOC on predicted θ_{PWP} , θ_{FC} , and θ_{AWHC} are not constant across soil texture classes (Table 3). For noncalcareous soils, the effect of increasing SOC is most prominent in θ_{AWHC} , because of the combined effects at θ_{PWP} and θ_{FC} . This absolute effect is largest for fine textured soils. For example, changes in θ_{AWHC} due to increased SOC for fine textured soils is 30% greater relative to the mean of all textures, and coarse soils are 30% less relative to the mean of all textures. In calcareous soils, because SOC has no interaction term with texture for θ_{PWP} , the effect of increasing SOC is only in θ_{FC} . Coarse-textured calcareous soils have twice the water retention due to increased SOC compared with the mean of all textures (Table 3). Previous findings have shown that the magnitude of change resulting from increases in SOC was greatest in coarse-textured soil and least in fine-textured soils for θ_{PWP} , θ_{FC} , and θ_{AWHC} (Hudson, 1994; Minasny & McBratney, 2018). Our findings agree with past literature for the repacked cores used to make new θ_{PWP} pedotransfer functions, but our findings are not consistent with the literature for noncalcareous soils for either θ_{FC} or θ_{AWHC} . The differences between our study and previous work are likely caused by differences in procedures, especially (a) the experimental design of the NAPESHM dataset was developed to capture changes in SOC and water retention due to management (treatment) effects within sites as well as across sites; (b) previous studies combined calcareous and noncalcareous soils, but we separate them; and (c) differences in the θ_{FC} measurement methodology from some past studies.

Increases in SOC can in some cases result in small reductions in predicted water content for the new pedotransfer functions. For noncalcareous soils, there was one simulated example of a silt (sand and clay at 5%) in which predicted θ_{PWP} decreased with more SOC (Table 3). This negative prediction was smaller than the RMSE (Equation 2) and is represented as the minimum value for noncalcareous θ_{PWP} predictions in medium textures soils in Table 3. For calcareous soils, there were 25 simulated examples that resulted in negative predicted changes in water content when SOC increased and these contributes to the negative values in Table 3 for calcareous soils. All were less than one-third of the RMSE for their respective equations. Thus, the new pedotransfer functions can predict small decreases in water content as the result of increased SOC. Given that the magnitude of these predictions is less than the RMSE of the equations, users may choose to interpret them as no change in water content.

TABLE 3 Summary statistics for the effects of increase in soil organic C for predicted volumetric water content at permanent wilting point (θ_{PWP}), field capacity (θ_{FC}), and plant available water holding capacity (θ_{AWHC}) using the new pedotransfer functions on simulated data. For calcareous soils $n = 270$ and for noncalcareous soil $n = 384$. Particle size group, clay, sandy clay, silty clay, clay loam and silty clay loam are fine; loam, silt loam, silt, and sandy clay loam are medium; and sand, loamy sand, and sandy loam are coarse

Particle size group	Change in water content (mm 100 mm ⁻¹) from 10 g kg ⁻¹ Increase in soil organic C		
	Min.	Mean	Max.
Noncalcareous			
θ_{PWP}			
Coarse	0.9	1.5	1.9
Medium	-0.1	0.8	1.9
Fine	0.5	1.3	1.9
All	-0.1	1.2	1.9
θ_{FC}			
Coarse	2.8	4.2	5.2
Medium	0.5	3.1	5.9
Fine	2.6	5.1	7.0
All	0.5	4.1	7.0
θ_{AWHC}			
Coarse	1.9	2.7	3.4
Medium	0.6	2.2	4.0
Fine	2.1	3.8	5.0
All	0.6	3.0	5.0
Calcareous			
θ_{PWP}			
Coarse	0.5	0.5	0.5
Medium	0.5	0.5	0.5
Fine	0.5	0.5	0.5
All	0.5	0.5	0.5
θ_{FC}			
Coarse	3.0	4.1	5.6
Medium	-0.2	1.7	3.3
Fine	-0.9	0.2	1.2
All	-0.9	2.0	5.6
θ_{AWHC}			
Coarse	2.5	3.6	5.2
Medium	-0.7	1.2	2.9
Fine	-1.3	-0.3	0.8
All	-1.1	1.5	5.2

For noncalcareous soils across texture classes, the increase in θ_{AWHC} associated with a 10 g kg⁻¹ increase in SOC ranged from 3.0 to 5.0 mm 100 mm⁻¹ (Table 3). In calcareous soils, predicted changes in θ_{AWHC} from a 10 g kg⁻¹ increase on SOC were smaller on average, but some larger changes were pre-

dicted. The range was 1.6–5.5 mm 100 mm⁻¹. For comparison to these predicted changes, the mean change in θ_{AWHC} associated with a 10 g kg⁻¹ increase in SOC reported by Minasny and McBratney (2018) was 1.2 mm 100 mm⁻¹ across all textures. Thus, the mean effect of SOC on θ_{AWHC} reported by Minasny and McBratney (2018) is about the same as our findings for calcareous soil and about a third as large as our findings for noncalcareous soils. We attribute the greater increase in predicted θ_{AWHC} for the new pedotransfer functions to the fact that NAPESHM data used to create the function captures variance in SOC and measured θ_{AWHC} within pedons due to management practices. Another source of improvement may be the somewhat larger sample size for measures θ_{FC} ; the intact clods used by Saxton and Rawls (2006) would have been approximately 8 × 6 × 6 cm so that they would fit snugly in the clod box (Soil Science Division Staff, 2017). The volume of a soil clod fitting in a clod box is approximately 72–78% of the volume of the core used in this investigation.

This study demonstrates that, while there are cases in which the magnitude of change in θ_{AWHC} resulting from increased SOC will be negligible, other cases will show meaningful benefits of increasing SOC. To illustrate how these changes might be meaningful to crop production, a fine-textured soil with a 20 g kg⁻¹ increase in SOC would increase θ_{AWHC} by 7.6 mm 100 mm⁻¹ (Table 3). Extending this to 150-mm depth would result in 11.4 mm of additional plant available water. Assuming that plants took up this 11.4 mm of additional water and that it was recharged in five rainfall events throughout a growing season, the additional water available to plants over the growing season would be 57 mm (2.2 in, 570,000 L ha⁻¹ yr⁻¹). For reference as to whether this may be a meaningful increase, an estimate for the amount of water that corn needs for transpiration during the reproductive phase is about 5 mm per day. To determine whether increases in θ_{AWHC} are meaningful to stakeholders, considerations such as rainfall amount and timing and planting and harvesting of crops should inform situational analysis. This study enables such situational analyses by making available new pedotransfer functions for θ_{PWP} , θ_{FC} , and θ_{AWHC} that meaningfully respond to changes in SOC that result from soil management.

4 | CONCLUSIONS

The newly developed pedotransfer functions for soil water retention have similar performance compared with previous models and is more sensitive to changes in SOC. The new functions provided robust estimates for 1,731 surface soils from the NCSS database. The magnitude of predicted increases in θ_{PWP} , θ_{FC} , and θ_{AWHC} in response to increased SOC was greater for noncalcareous soils, which showed a mean increase in θ_{AWHC} across all texture classes that was more than double that reported in earlier studies. The

accuracy of new functions provides confidence that they are suitable to incorporate into models. Because they demonstrate a change in response to varying levels of SOC, they bridge the long-standing discrepancy between soil science textbooks and pedotransfer functions on the effects of SOC on θ_{AWHC} .

While there was broad representation in soil types in the NAPESHM dataset used to develop the new pedotransfer functions, there were some conditions with limited data to train the model. For example, the functionality of the new pedotransfer function for noncalcareous soil is limited to no more than 60% clay. This study highlights the need for more mechanistic investigation and pedotransfer function development to understand water retention in calcareous soils.

The newly developed pedotransfer functions show substantial effects of SOC on θ_{AWHC} and will enable future modeling to illuminate scenarios for which changes in soil management that result in increased SOC are likely to provide changes in water supplied to plants by the soil that are meaningful for stakeholders.

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CONFLICT OF INTEREST

The authors declare no conflict of interest.

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