ESTIMATING SOIL QUALITY INDICATORS WITH DIFFUSE REFLECTANCE SPECTROSCOPY

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ABSTRACT

Knowledge of within-field spatial variability in soil quality indicators is important to assess the impact of site-specific management on the soil. Standard methods for measuring these properties require considerable time and expense, so sensor-based approaches would be useful. The purpose of this research was to evaluate the ability of visible and near infrared (VNIR) diffuse reflectance spectroscopy (DRS) to estimate soil properties that are candidate soil quality indicators. Soil samples were obtained from two depths (0-5 and 5-15 cm) at a long-term (since 1991) experimental site in central Missouri where cropping systems were replicated across a typical claypan soil landscape. Laboratory analyses were conducted for potential indicators of soil quality, including soil organic carbon, soil glucosidase enzyme activity, and plant available nutrients. VNIR-DRS data were obtained in the laboratory using a spectrometer with a wavelength range of 350 to 2500 nm and calibrations to soil properties were developed with partial least squares regression. Results showed that VNIR DRS has potential to estimate several key soil quality indicators (SQI), including soil organic carbon, total soil nitrogen, glucosidase activity, and pH. However, other key SQI, such as aggregate stability, plant available nutrients, and nitrate and ammonia forms of nitrogen were not successfully estimated by this technology. Thus, a sensor fusion approach, combining VNIR DRS with other technologies, would likely be needed for implementing a sensor-based soil quality index.

Keywords: soil quality, diffuse reflectance, near-infrared, spectroscopy

INTRODUCTION

The soil quality concept involves the capacity of a soil to function; included among the soil functions are water flow and retention, physical stability and support, retention and cycling of nutrients, and maintenance of biodiversity, habitat, and crop productivity (Karlen et al., 1997). Best management practices (BMPs) to improve soil quality encompass an array of strategies, including reduced or no tillage, crop rotation, reduced chemical inputs, and more efficient use of chemical inputs, such as may be found with variable rate application (Larson et al., 1997).

Evaluation of management impacts on soil quality is based on measurement of soil quality indicators (SQI) (Doran and Parkin, 1996). Soil organic matter (SOM), because of its integral role in soil biological, physical, and chemical processes, is usually considered to be the quintessential SQI (Carter, 2002). Measurements of SQI generally involve field collection of soil samples and laboratory analysis. The labor and expense involved make this approach more suited to research investigations than to monitoring production fields because many SQI can exhibit strong spatial dependence at the field scale (Cambardella et al., 1994; Jung et al., 2006), requiring dozens or hundreds of measurements per field for good representation. To transfer the soil quality approach to practice, methods that can efficiently map SQI across fields and landscapes are needed.

Diffuse reflectance spectroscopy (DRS) is a method that has been successfully used to estimate soil organic carbon (SOC), SOM, and numerous other properties related to soil quality (see reviews by Malley et al., 2004; Viscarra Rossel et al., 2006; Stenberg et al., 2010). Most commonly, soil sensing by DRS uses the visible (400–700 nm), near-infrared (NIR; 700–2500 nm), or combined VNIR (400–2500 nm) wavelength ranges. This method is based on the interaction of light with the surface at which it is directed. Characteristics of the reflected light are influenced by the chemical and physical properties of the target, such that these properties can be estimated through statistical analysis of the reflectance spectrum (Malley et al., 2004).

Several researchers, with the specific goal of soil quality assessment in mind, have used VNIR spectroscopy to estimate various SOM components. Vasques et al. (2009) estimated four organic C fractions (in order of decreasing residence time in soil) – recalcitrant C, hydrolyzable C, hot-water-soluble C, and mineralizable C. Using samples obtained across a north-central Florida watershed, VNIR models accounted for from 65 to 82% of the variation present in a validation dataset. Pietikäinen and Fritze (1995) used NIR data to estimate microbial biomass C, accounting for 74 to 82% of the variance in that variable for samples from an experimental forest in Finland. Ludwig et al. (2002) used VNIR analysis to estimate chemical and biological properties related to soil sustainability. They found good results for C, N, microbial C, and a number of other variables. Chang et al. (2001) related VNIR data to a range of chemical and biological soil properties. Among the properties with the strongest relationships to the VNIR data were C, N, and biomass C. Good VNIR or NIR estimates have also been obtained for humic acid fractions (Butkuté and Šlepetiené, 2006), and for particulate organic matter (POM) and POM-C (Reeves et al., 2006; Sheridan et al., 2011).

Others have related VNIR or NIR reflectance to more general soil quality indices. Cécillon et al. (2009) modeled soil quality using three indicators related to organic matter, nutrient supply, and biological activity. They found that NIR reflectance was strongly related to those indicators ($r^2 \geq 0.9$) over a wildfire chronosequence in a Mediterranean forest ecosystem. Palmborg and Nordgren (1996) used NIR measurements together with heavy metal concentration data to help explain differences in microbial parameters, assuming that the NIR data were related to “organic matter quality.”

Although prior research has documented the ability of VNIR DRS to estimate variations in SQI, these studies have often drawn samples from a wide geographic area (i.e., 100s of km^2 or more) or from non-agricultural areas such as forests. Few have investigated the ability of VNIR reflectance to estimate differences in soil quality variables across landscapes within an agricultural field.

Objectives

The objective of this research was to evaluate VNIR DRS for within-landscape estimation of soil properties that are candidate soil quality indicators. These included soil properties (e.g., SOC) successfully estimated by VNIR DRS in previous studies along with others (e.g., soil glucosidase activity, water stable aggregates) to which VNIR DRS had not been previously applied.

MATERIALS AND METHODS

Study Site and Sample Collection

The study was conducted on a 12-ha site 2 km from Centralia, Missouri (39˚13 N, 92˚07 W). The site is in Major Land Resource Area 113, the Central Claypan Region (USDA-NRCS, 2006), which covers 33,000 km^2 in the states of Missouri and Illinois. The site encompasses three landscape positions: summit, backslope and footslope (Fig. 1). Soils were delineated on the basis of an order-one soil survey conducted in 1991 (Fig. 1). The difference in elevation between summit and footslope positions was about 2-3 m. The distinguishing factor of the soils at the site is the namesake “claypan.” The claypan is an abrupt textural discontinuity, serving as the upper boundary of an argillic horizon having at least 100% more clay than in the horizon above. This claypan commonly contains as much as 50 to 60% smectitic clay, and is followed by a series of argillic horizons with decreasing clay content. These strongly affect water infiltration and soil water holding capacity.

Variations in soil quality were expected across the site due to the four rotational grain cropping systems and one perennial grass system established in 1991 to investigate the effects of tillage (i.e., minimum tillage vs. no-tillage), crop rotation, and other management practices (e.g., cover crops) on crop production and soil and water quality. The experimental design was a randomized complete block with three blocks (i.e., replications) where all rotation phases of each cropping system were present each year. Each of the 30 plots measured 18 m × 189 m (0.35 ha) running east-west parallel to the slope direction (Fig. 1) and thus each landscape position was included within each plot. In 2001 the three grass cropping system plots were split into thirds lengthwise and two additional grass systems were established. Background soil profile data obtained from the experimental area in 1991 are described by Jung et al. (2010). Descriptions of management systems are given in Chaudhary et al. (2012).

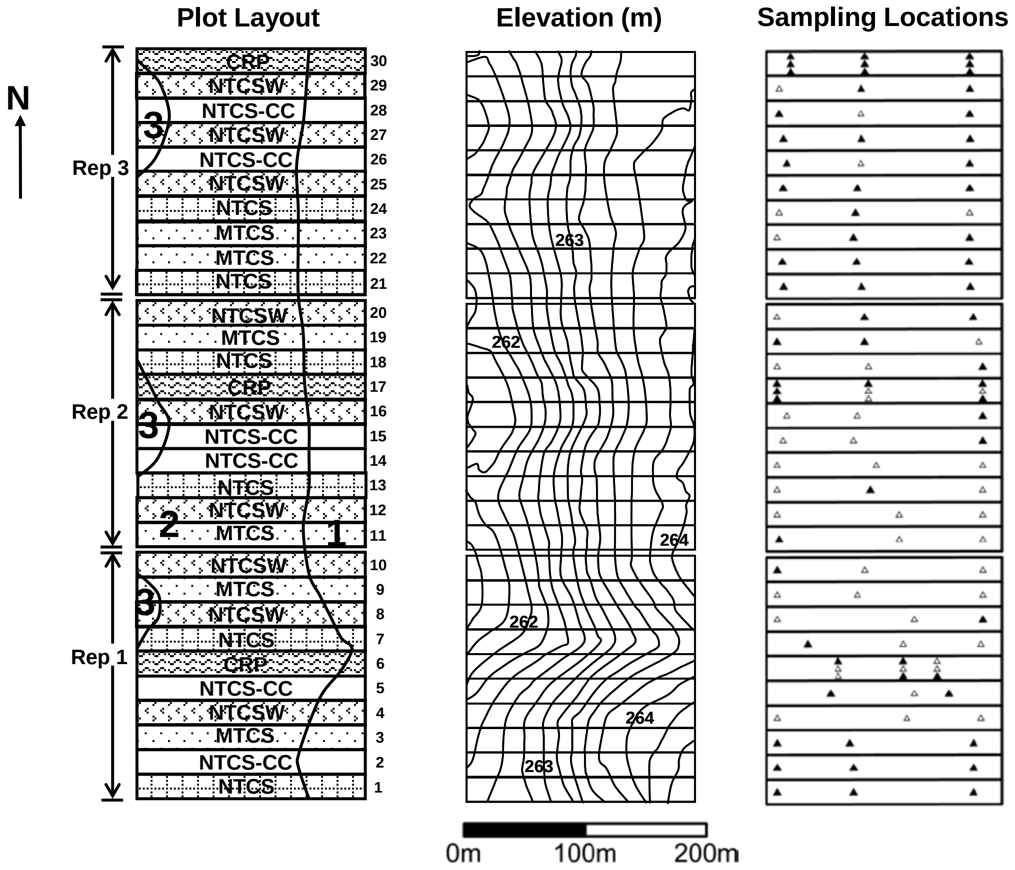

Fig. 1. Site layout with soil series, cropping systems, elevation, and sampling points. Soils: 1-Adco silt loam, 0-1% slope; 2-Mexico silty clay loam, 1-3%, eroded; 3-Mexico silt loam, 1-2%. Cropping systems: MTCS = mulch tillage corn-soybean rotation; NTCS = no-till corn-soybean; NTCSW = no-till corn-soybean-wheat rotation; NTCS-CC = no-till corn-soybean with cover crops; CRP = conservation reserve program. CRP plots were further split in thirds lengthwise for the three grass cropping systems of this study.

Soil samples were obtained in the fall of 2010 at predefined locations within each plot, centered on each of the three landscape positions (Fig. 1). At each location, three sub-sample points were established in a triangular arrangement within a 3-m radius to obtain an average representative of the location. Three 3.2-cm diameter cores were obtained at each of the sub-sample points. The cores were divided into two depth increments, 0-5 cm and 5-15 cm, and the nine total samples were bulked to represent each landscape position. Cores were distributed evenly across row positions to equally sample between and within row effects. Samples were sealed in plastic bags and stored at 4° C prior to processing.

Laboratory Soil Analysis

Soil samples were analyzed in the laboratory for plant available nutrients and several established SQI. Macro and micronutrient content was quantified by Mehlich III extraction (Mehlich, 1984) followed by analysis using inductively coupled plasma–atomic emission spectrophotometry (Soltanpour et al., 1996). Total nitrogen (TN) and SOC were determined by dry combustion at 900°C (Nelson and Sommers, 1996) on a LECO Tru-Spec C/N analyzer (LECO Corp., St. Joseph, MI) using an infrared detector for CO_2 gas and a thermal conductivity detector for N_2 gas generated by the process.

Water-stable aggregates (WSA) were determined on 10-g air-dried soil samples using a wet-sieving method (Angers and Mehuys, 1993; Kemper and Rosenau, 1986). Soil samples were spread on a 250- µm sieve, placed on the wet-sieving apparatus and subjected to periodic immersion in water (30 vertical strokes/min for 10 min). Soil particles that passed through the sieve were considered the fraction that was unstable in water. Soil remaining on the sieve was dried at 105°C, weighed and dispersed with 50 ml of 0.5% sodium hexa-metaphosphate to separate water-stable soil fractions from coarse particles. Coarse particles were collected, dried and weighed. The proportion of WSA was calculated as a percentage of the weight of the stable fraction of the total soil weight.

Soil microbial activity is often represented as the activity determined for selected soil enzymes. For this study, ß-glucosidase activity (GluAct), indicative of carbon mineralization, was determined by incubating 1-g soil samples with *p*-nitrophenyl- ß-D-glucoside substrate for 1 h at 37°C (Dick et al. 1996). After incubation, reaction mixtures were filtered and the concentration of the product, *p*-nitrophenol (PNP), was determined spectrophotometrically at 410 nm and the enzyme activity expressed as µg PNP released g^{-1} dry soil h^{-1}.

Spectral Data Collection and Processing

Soil spectral reflectance data were obtained in the laboratory using an ASD FieldSpec Pro FR spectrometer (Analytical Spectral Devices, Boulder, CO). For reflectance data collection, subsamples of the soils collected in the field were oven dried and sieved with a 2-mm screen. Approximately 15 cm^3 of soil was packed in a glass-bottomed sample cup. The sample was illuminated through the glass by a halogen lamp and the reflected light from an approximately 12 mm diameter area was transmitted to the spectrometer through a fiber optic bundle. Spectra recorded between 350 and 2500 nm were output on a 1-nm interval. Each soil spectrum was obtained as the mean of 30 scans. The spectrometer data collection software automatically adjusted the data for dark current variations using dark current scans obtained at the beginning of each data collection session, and at least once every 30 minutes thereafter. A Spectralon (Labsphere Inc., North Sutton, N.H.) reflectance standard was scanned after every five soils and used to convert the raw spectral data to decimal reflectance. Spectra were obtained in triplicate by rotating the sample cup approximately 60 degrees between scans, and averaged to a single spectrum per each sample for analysis.

Data analysis was carried out in Unscrambler version 10.1 (CAMO Inc., Oslo, Norway). First, readings below 400 nm were deleted due to their low signal-to-noise ratio. Next, the effects of several spectral transformations and combinations were investigated in a preliminary analysis. Best results were obtained using the “de-trending” transformation in Unscrambler that used a second-order polynomial to remove baseline shift effects from the spectra (CAMO, 2006). Therefore, all spectral data were subjected to this transformation before regression analyses.

Partial least squares (PLS) regression was used to develop calibrations between soil properties and spectra. A 20-fold cross validation procedure was used to select the number of PLS factors to use in the regression, increasing predictive capability and decreasing the potential for overfitting. Model evaluation was based on coefficient of determination (R^2), root mean square error of prediction (RMSEP), and the ratio of standard deviation to RMSEP (RPD). RPD is useful when comparing results from datasets containing different degrees of variability. Chang et al. (2001) suggested that, as a general guideline, RPD > 2.0 or $R^2 > 0.8$ indicates success in estimating soil properties, RPD < 1.4 or $R^2 < 0.5$ shows unacceptable results, and calibrations with intermediate values may be improved to acceptable levels using different strategies.

RESULTS AND DISCUSSION

Table 1 shows descriptive statistics for the laboratory soil analysis. The management systems at the study area imposed a wide variation in values of most soil properties. Of the 21 measured, only two (Na and pH) had a coefficient of variation (CV) less than 20%. Three additional properties (C:N ratio, WSA, and Fe) had CV less than 30%. Although a high CV does not necessarily imply success, soil properties with a low CV generally are not well-estimated by VNIR DRS.

Correlations among the laboratory-measured soil properties were examined. Of the 210 variable pairs, only 28 (13%) exhibited a Pearson correlation coefficient (r) above 0.4. Of these, there were only 4 pairs with r > 0.7 – Mg and Ca; SOC and TN; SOC and GluAct; and TN and GluAct.

PLS regressions estimating soil quality properties as a function of VNIR spectral data gave mixed results (Table 2). Consistent with many reports in the literature (e.g., Lee et al., 2009; Sheridan et al., 2011), best results were obtained for SOC. Regressions for TN and GluAct also gave good results, with $R^2 > 0.65$. Accuracy of SOC and TN estimations were very similar to those reported for a subset of these same plots based on a 2008 sampling campaign (Chaudhary et al., 2012). In that study, management and landscape differences in SOC and TN were detected by VNIR DRS data, although with somewhat less power than data from standard laboratory analysis. Thus, we would also expect the SQI data of this study to detect soil quality differences among the treatments at the study site.

The strong correlations between SOC, TN, and GluAct might suggest that results for TN and GluAct were not from a direct estimation of those properties by VNIR DRS, but rather an indirect effect of their correlation with SOC. However, Chang and Laird (2002) spiked soil samples to change C:N ratio from what would be expected in nature and found that TN was still well estimated, leading them to conclude that VNIR estimation of TN was through a direct calibration in their study. Stott et al. (2010) noted little relationship between SOC and GluAct for a wide range of soils and cropping systems, but noted that such relationships might be stronger within a given location. Thus, it is possible that the GluAct calibration is an indirect one, which would make it less likely to be transferrable to other datasets. Further research with a diverse set of soil samples from multiple locations could potentially help resolve this issue.

The only soil fertility properties estimated with good accuracy were pH (R^2 = 0.69) and Mg (R^2 = 0.64), with all others having $R^2 \leq 0.41$. Similarly, Sudduth et al. (2010) found that VNIR DRS estimates of pH and Mg were better than those of other soil fertility properties on a nearby field with soils similar to those of the study site. Generally, trends in estimation accuracy among the macronutrients followed those reported in other studies, including Lee et al. (2009). Estimates of micronutrients were poor, with $R^2 < 0.4$ in all cases. Few previous studies are available for comparison, but our results were generally poorer than those reported for several micronutrients by Chang et al. (2001). In contrast to our study, where samples were all from a 12 ha area, their data came from over 800 soil samples obtained from across the US.

Table 1. Descriptive statistics for laboratory-measured soil properties.

Property	Mean	SD	Min	Max
Soil Quality				
Glucosidase activity, mg kg^{-1} h^{-1}	96.9	51.5	17.2	247.2
SOC, g kg^{-1}	16.87	6.36	8.99	41.90
TN, g kg^{-1}	1.69	0.53	0.81	3.62
C:N Ratio	9.9	2.1	3.0	29.3
Water stable aggregates, %	67.1	16.4	11.5	88.8
Soil Fertility				
pH	6.3	0.4	4.7	7.0
B, mg kg^{-1}	0.27	0.28	0.00	1.11
Ca, mg kg^{-1}	2129	842	313	5931
Co, mg kg^{-1}	0.22	0.19	0.00	1.61
Cu, mg kg^{-1}	0.52	0.30	0.00	1.98
Fe, mg kg^{-1}	71.4	20.9	13.0	149.7
K, mg kg^{-1}	83.4	48.4	15.1	353.2
Mg, mg kg^{-1}	244	151	39	1035
Mn, mg kg^{-1}	21.5	8.4	1.5	49.7
Mo, mg kg^{-1}	0.014	0.039	0	0.277
Na, mg kg^{-1}	388	61	41	527
NH_4, mg kg^{-1}	0.17	0.38	0.00	3.91
Ni, mg kg^{-1}	0.23	0.34	0.00	2.86
NO_3, mg kg^{-1}	2.65	3.26	0.10	21.10
P, mg kg^{-1}	11.11	8.44	0.00	41.69
Zn, mg kg^{-1}	8.05	6.48	0.50	39.83

Table 2. Partial least squares (PLS) regression cross-validation statistics. Units for RMSEP and bias are found in Table 1.

Property	NF*	R^2	RMSEP	RPD	Slope	Bias
Soil Quality						
Glucosidase activity	6	0.66	30.2	1.71	0.669	32.1
SOC	8	0.84	2.55	2.49	0.847	2.58
TN	11	0.69	0.283	1.87	0.738	0.443
C:N Ratio	9	0.18	1.39	1.50	0.262	7.28
WSA	5	0.16	15.0	1.09	0.240	50.9
Soil Fertility						
pH	7	0.69	0.245	1.80	0.711	1.83
B	No PLS regression solution achieved					
Ca	6	0.36	673	1.25	0.407	0.0013
Co	1	0.06	0.187	1.03	0.0678	0.200
Cu	5	0.22	0.265	1.13	0.250	0.391
Fe	6	0.15	19.0	1.10	0.215	56.4
K	8	0.41	37.2	1.30	0.463	45.3
Mg	6	0.64	87.7	1.72	0.654	83.0
Mn	10	0.38	6.63	1.27	0.462	11.6
Mo	1	0.02	0.0388	1.01	0.0223	0.0137
Na	10	0.15	51.6	1.18	0.211	307
NH_4	3	0.01	0.377	1.00	0.0177	0.169
Ni	4	0.13	0.319	1.08	0.149	0.194
NO_3	4	0.09	3.13	1.04	0.114	2.35
P	6	0.33	6.95	1.21	0.360	7.10
Zn	2	0.15	6.02	1.08	0.153	6.83

* NF = number of PLS factors used in the model; RMSEP = root mean standard error of prediction; RPD = standard deviation /RMSEP.

SUMMARY

The ability of VNIR DRS data to estimate soil quality and soil fertility properties across farming systems was investigated. Most laboratory-measured soil properties were strongly variable across the study area, as a consequence of approximately 20 years of differential management. VNIR DRS provided very good estimates of SOC, and good estimates of TN and GluAct. Further investigation is warranted to determine if GluAct estimations are a direct spectral response or are due to a strong correlation with SOC. Relative accuracy of soil fertility estimates generally followed previously reported results, with pH and Mg providing the best results.

These results show that VNIR DRS has potential to estimate several key SQI, including SOM, TN, microbial activity (i.e., GluAct), and pH. However, other key SQI, such as aggregate stability, plant available nutrients, and other N forms were not successfully estimated by this technology. Thus, a sensor fusion approach combining VNIR DRS with other technologies would likely be needed for implementing a sensor-based soil quality index.

ACKNOWLEDGEMENTS AND DISCLAIMER

We acknowledge the following for assistance in data collection, processing and analysis: Scott Drummond, Bob Mahurin, Kurt Holiman, Matt Volkmann, Jim Ortbals, Eric Allphin, Alec Sheridan, and Anna Hodge.

Mention of trade names or commercial products in this paper is solely for the purpose of providing specific information and does not imply recommendation or endorsement by the United States Department of Agriculture.

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