VNIR Spectroscopy Estimation of Soil Quality Indicators

Kenneth A. Sudduth, Agricultural Engineer
Newell R. Kitchen, Soil Scientist
Robert J. Kremer, Microbiologist
USDA-ARS Cropping Systems and Water Quality Research Unit, Columbia, Missouri

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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 purposes of this research were (1) to evaluate changes in soil quality indicators after initiation of a precision conservation system on a typical claypan-soil research field in northeast Missouri and (2) to evaluate the ability of visible and near infrared (VNIR) spectroscopy to estimate those soil quality indicators. Soil samples were obtained to a 15-cm depth on a 30-m grid spacing, plus at a number of random sampling locations, before and three years after conversion from a corn-soybean rotation to a no-till soybean-wheat-hay rotation. Laboratory analyses were conducted for potential indicators of soil quality, including chemical constituents, labile and total organic carbon, and particulate organic matter carbon (POM-C) and nitrogen (POM-N). VNIR reflectance of dried and sieved samples was obtained in the laboratory using a spectrometer with a wavelength range from 350 to 2500 nm. Calibrations of VNIR reflectance to soil quality parameters were accomplished using partial least squares regression. Laboratory analysis showed a significant increase in soil quality indicator values over the study period, particularly POM-C and POM-N. These increases were greatest in the wetter, lower-landscape portions of the field, perhaps due to higher biological activity. VNIR spectroscopy was not able to accurately estimate the soil variables studied, with the exception of pH. This may have been due to their relatively low variability across the study area. Further research will evaluate VNIR spectroscopy for estimating soil quality indicators across multiple management systems where variability is expected to be greater.

Keywords. Soil quality, VNIR spectroscopy, soil organic carbon
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; Andrews et al., 2004). The concept of soil quality not only includes sustaining crop productivity but also maintaining environmental quality, and it is likely that enhancement of soil quality would be a major barrier against degradation of water and air quality (Kennedy and Papendick, 1995). 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 (SQIs) (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). Although SQIs most directly portray the current state of management systems, soil quality assessments using selected SQIs are perhaps most valuable to further improve future, sustainable land management practices. Thus, SQIs that are sensitive to short-term (i.e., a few years) changes in soil quality due to management are desirable so that the effects of improved management can be documented in a relatively short time.

Soil organic carbon (SOC, the carbon content of SOM) is a standard laboratory measurement used in SQIs. However, Wander et al. (1994) concluded that total SOC was not suitable for tracking changes in soil fertility occurring during a 3-4 yr transition period following conversion to organic management. Biologically active SOM fractions are important for nutrient cycling and supply and may be controlled more by management than total SOC. Therefore, detection and quantifying sensitive or responsive fractions such as particulate organic carbon (POM-C, the carbon content of particulate organic matter, or POM) might provide better insight on the effects of management changes (Franzluebbers and Stuedemann, 2008; Marriott and Wander, 2006). This is because POM is composed of partially decomposed plant, animal, and microbial residues, serves as a readily available energy source for soil microorganisms, and is related to indices of N supply and nutrient cycling.

Measurement of C released by oxidation of soil with potassium permanganate (KMnO₄) is considered by many as a means of quantifying labile C in soils. Although most procedures are based on 333 mM KMnO₄ extractant, Weil et al. (2003) proposed a modified method using 20 mM KMnO₄ which quantified an active SOC pool that correlated highly with microbial respiration, microbial biomass, and soluble carbohydrates, more so than C pools identified with 333 KMnO₄. Recent research suggested that permanganate oxidizable C (MnOxC) is influenced by total SOC, soil texture, and C content of organic materials added to soil, and thus may not be a sensitive indicator of labile C (Tirol-Padre and Ladha, 2004). Mirsky et al. (2008) similarly concluded that MnOxC responded significantly to organic additions to soil; however, because it was significantly correlated with POM, they suggested that MnOxC, with further method development, had high potential as a reliable soil quality assessment tool. Skjemstad et al. (2006) reported that MnOxC was sensitive to the presence of lignin or lignin-derived SOC, but did not seem to be sensitive to changes in SOC under long-term management.

A significant contribution of soil quality assessments is translating information into practical tools and strategies that land managers can use to evaluate the sustainability of agroecosystem and natural ecosystem management practices. However, the use of such assessments is often limited by the cost and complexity of the laboratory analyses required. One potential way to address this issue would be by replacing laboratory analyses with spectroscopic data collection.
Visible-near-infrared (VNIR) and mid-infrared (MIR) reflectance spectroscopy have both been used for estimation of a number of soil properties (Sudduth et al., 1997; Viscarra Rossel et al., 2006).

Much VNIR soil property research has investigated SOC or SOM (Viscarra Rossel et al., 2006), quantities which are of direct importance in soil quality assessment. 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 Šlepetienė, 2006), and for POM and POM-C (Reeves et al., 2006).

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 reflectance to estimate variations in soil C fractions and other soil quality variables, these studies have generally drawn samples from a wide geographic area (i.e., 100s of km\(^2\) or more) or from non-agricultural areas such as forests. Research on the ability of NIR to estimate temporal or spatial differences in soil quality variables within a single field is lacking.

**Objectives**

The primary objective of this study was to quantify the ability of VNIR spectroscopy to estimate variability in selected soil quality indicators within a typical production field in central Missouri. A secondary objective was to evaluate the differences in laboratory-measured soil quality indicators before and after conversion of the field from a conventional corn-soybean production system to a conservation-oriented precision agriculture system.

**Materials and Methods**

**Study Site and Soil Sampling**

Data were collected on a 35-ha research field located near Centralia, Missouri (92.12 E, 39.97 N). Soils are claypan soils of the Mexico (fine, smectitic, mesic aeric Vertic Epiaqualfs) and Adco (fine, smectitic, mesic aeric Vertic Albaqualfs) series. Surface textures range from silt loam to silty clay loam. The subsoil claypan horizon(s) are silty clay loam, silty clay, or clay, and commonly contain as much as 50 to 60% smectitic clay.
The study field, historically managed in a corn-soybean rotation, had been intensively monitored for water quality and for spatial variation in soil properties, crop yields, and other parameters since the early 1990s. This detailed information was used to develop a precision agriculture system (PAS) plan for the field as described by Kitchen et al. (2005) and Lerch et al. (2005). Implementation of the PAS plan began in 2004 and promising preliminary results have been reported (Sudduth et al., 2007).

To capture soil differences before and after PAS implementation, we sampled the field on a 30-m grid to a 15-cm depth in the spring of 2003 and spring of 2007. Additional samples were obtained at random locations to help define the short-range spatial structure. At each grid point, eight 1.5-cm diameter cores were obtained to a 15-cm depth and composited. For this study, we used samples from a 7 ha subarea of the field to reduce the cost and labor associated with laboratory analysis, resulting in 104 soil samples for each year.

**Laboratory Analysis**

Samples were analyzed for soil fertility, organic carbon and nitrogen. Measurements of soil fertility – P (Bray 1 extractable), K, and pH – were carried out using standard University of Missouri procedures (Nathan et al., 2006).

Total SOC and total N were determined with dry combustion (900ºC) using a LECO Tru-Spec C/N Analyzer1 (LECO Corp., St. Joseph, Mich.) on soil subsamples dried at 60ºC. Soil pH was <6.8, thus total C was considered equivalent to organic C. Accuracy of analyses for determinations on all samples was ±0.06% C and ±0.019% N.

Laboratory analysis of POM followed methods of Cambardella and Elliott (1992) and Marriott and Wander (2006). We used 25 g dry soil, dispensed in 50-mL centrifuge tubes and shaken with 30 mL of 5% sodium hexametaphosphate for 2 h on a reciprocal shaker at approximately 180 oscillations per min. The suspension was passed through a 53-µm sieve and rinsed with distilled water until a clear solution was obtained. Material retained on the sieve, a mixture of sand and POM, was carefully transferred into flasks and dried at 60ºC. The dried material was weighed, ground with mortar and pestle, and analyzed for C (POM-C) and N (POM-N) using the combustion method described above.

Chemically labile MnOxC was analyzed following the procedure of Weil et al. (2003). Dried soil samples weighing 5 g were added to 50-mL plastic screw-cap centrifuge tubes. Soil was reacted with 20 mL of 20 mM KMnO₄ prepared in 100 mM CaCl₂. The soil was shaken on a rotary shaker for 2 min at 180 rpm and allowed to settle for 10 min. A 200-µL aliquot of the supernatant was diluted to 10 mL and absorbance was measured spectrophotometrically at 550 nm. The amount of C oxidized after digestion was based on a standard curve using the assumption that 9 mg C is oxidized for every 4 mmoles of Mn⁺⁷ that are reduced (Weil et al., 2003).

**Spectral Data Acquisition and Analysis**

Soil spectral reflectance data were obtained in the laboratory using an ASD FieldSpec Pro FR spectrometer (Analytical Spectral Devices, Boulder, Colo.). For reflectance data collection, subsamples of the soils collected in the field were air dried and sieved with a 2-mm screen. Approximately 15 cm³ of soil was packed in a glass-bottomed sample cup for reflectance

1 Mention of trade names or commercial products is solely for the purpose of providing specific information and does not imply recommendation or endorsement by the US Department of Agriculture.
determination. 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 10 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 10 soils and used to convert the raw spectral data to decimal reflectance. Spectra were obtained in either duplicate (2003) or triplicate (2007).

Reflectance data were preprocessed to remove erroneous measurements and improve stability of the regression. The first 100 readings at the lower visible wavelengths were deleted due to their low signal-to-noise ratio; thus the revised spectra began at 450 nm. Then, each spectral scan was (1) transformed from reflectance to absorbance (log10 [1/reflectance]), (2) mean-normalized (i.e., divided by its mean value), and (3) smoothed by applying a 10-point (10-nm) averaging, reducing the number of spectral variables to 205. Preliminary analyses had shown no improvement with other data transformations (e.g., derivative), so no other transformations were applied.

Partial least squares (PLS) regression, implemented in Unscrambler version 9.1 (CAMO Inc., Oslo, Norway), 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

Impact of PAS Implementation on Soil Properties

The PAS management implemented on this field in 2004 imposed different treatments on different portions of the field. For the portion sampled in this study, the plan adopted a no-till soybean-wheat-hay crop rotation (three crops in two years) instead of the soybean-corn rotation previously followed on the entire field. Winter annuals or perennials were used to maintain ground cover during winter and spring runoff events. We also expected the perennial plants grown with the hay crop to promote soil organic matter and aggregate stability and to lead to subsequent improvement in infiltration and reduced runoff.

Following three years of PAS, significant increases were observed in all measured soil parameters, with the exception of MnOxC, which decreased slightly (table 1). Mean values of pH, P, and K increased in the 7-ha study area. Similar increases in these fertility parameters, along with decreases in CV, were noted across the entire field as a consequence of variable-rate P, K, and lime application (Sudduth et al., 2007). We interpreted the significant increases in SOC, N, POM-C, and POM-N as indications that the cover crops implemented with PAS were achieving their desired goal of improving soil quality. Particularly notable was the 68% increase in POM-C from 2003 to 2007, as POM is considered to be the more biologically active portion of SOM and should respond more quickly to changes in management.
Table 1. Means and standard deviations of laboratory measured soil properties.

<table>
<thead>
<tr>
<th>Property and units</th>
<th>2003 Mean</th>
<th>Std. Dev.</th>
<th>2007 Mean</th>
<th>Std. Dev.</th>
</tr>
</thead>
<tbody>
<tr>
<td>pH</td>
<td>6.18</td>
<td>0.46</td>
<td>6.34</td>
<td>0.33</td>
</tr>
<tr>
<td>P, mg/kg</td>
<td>7.6</td>
<td>3.0</td>
<td>15.1</td>
<td>7.8</td>
</tr>
<tr>
<td>K, mg/kg</td>
<td>60.9</td>
<td>12.3</td>
<td>133.6</td>
<td>48.3</td>
</tr>
<tr>
<td>SOC, g/kg</td>
<td>11.5</td>
<td>1.1</td>
<td>12.4</td>
<td>1.3</td>
</tr>
<tr>
<td>POM-C, g/kg</td>
<td>1.49</td>
<td>0.43</td>
<td>2.51</td>
<td>1.12</td>
</tr>
<tr>
<td>MnOxC, g/kg</td>
<td>0.344</td>
<td>0.002</td>
<td>0.342</td>
<td>0.002</td>
</tr>
<tr>
<td>Total N, g/kg</td>
<td>1.07</td>
<td>0.18</td>
<td>1.18</td>
<td>0.17</td>
</tr>
<tr>
<td>POM-N, g/kg</td>
<td>0.117</td>
<td>0.030</td>
<td>0.166</td>
<td>0.073</td>
</tr>
</tbody>
</table>

The differences in soil C and N variables from 2003 to 2007 exhibited differing degrees of spatial structure. Little if any spatial structure was seen in the difference maps of MnOxC and total N, while SOC had a moderate amount of structure (fig. 1). Strong spatial structure was seen in POM-N and POM-C. With POM variables, the largest increases were found in the lower portions of the landscape (fig. 1), with deepest topsoil and highest water holding capacity, and the smallest increases were on the eroded sideslope areas. Patterns in POM-N and POM-C were spatially similar to the 2003 corn yield map (fig. 2), where a water-limited growing season resulted in a much higher yield in the lower, wetter portions of the landscape. Yield variation in the other three intervening years was relatively low and with little spatial structure (data not shown). We theorized that higher POM-N and POM-C in the lower portions of the landscape may have been due to the presence of more crop residue and increased microbial action in that portion of the landscape where the soil would be more consistently moist.

Figure 1. Temporal difference maps of soil C and N variables, along with elevation map of the study site. Positive numbers represent an increase from 2003 to 2007.
Figure 2. Corn yield in 2003, with higher yields in the lower-elevation, wetter portion of the landscape (fig. 1) where increases in POM-C and POM-N were also high.

**VNIR Estimation of Soil Properties**

There was relatively little difference in soil reflectance across the study area, also little difference between years (fig. 3). This fact indicated that calibrations of reflectance to soil properties might be particularly challenging in this situation.

Figure 3. Mean and ±1 standard deviation reflectance curves for 2003 and 2007 samples, along with the difference between the two means.

In fact, this was the case, as PLS calibration and cross-validation statistics for estimation of soil quality variables across the study field were generally poor, with low RPD and $R^2$ (table 2). The only exception was pH, with RPD approaching 2 and $R^2 > 0.7$. Calibrations for POM-C and POM-N were somewhat better than those for the other C and N variables, but were still of marginal usefulness. Thus, it seems unlikely that VNIR reflectance spectroscopy will be useful for estimating minor, within-field variations in these SQIs across typical claypan-soil landscapes.
Table 2. Calibration and validation statistics for VNIR estimation of soil properties.

<table>
<thead>
<tr>
<th>Soil Property</th>
<th>Calibration R²</th>
<th>RMSEC</th>
<th>Number of PLS Factors</th>
<th>Validation R²</th>
<th>RMSEP</th>
<th>RPD</th>
</tr>
</thead>
<tbody>
<tr>
<td>pH</td>
<td>0.76</td>
<td>0.19</td>
<td>10</td>
<td>0.71</td>
<td>0.21</td>
<td>1.87</td>
</tr>
<tr>
<td>P, mg/kg</td>
<td>0.32</td>
<td>6.0</td>
<td>8</td>
<td>0.26</td>
<td>6.3</td>
<td>1.15</td>
</tr>
<tr>
<td>K, mg/kg</td>
<td>0.41</td>
<td>40.1</td>
<td>8</td>
<td>0.36</td>
<td>41.8</td>
<td>1.25</td>
</tr>
<tr>
<td>SOC, g/kg</td>
<td>0.25</td>
<td>1.10</td>
<td>6</td>
<td>0.21</td>
<td>1.12</td>
<td>1.12</td>
</tr>
<tr>
<td>POM-C, g/kg</td>
<td>0.50</td>
<td>0.74</td>
<td>8</td>
<td>0.45</td>
<td>0.77</td>
<td>1.35</td>
</tr>
<tr>
<td>MnOxC, g/kg</td>
<td>0.03</td>
<td>0.0022</td>
<td>2</td>
<td>0.02</td>
<td>0.0022</td>
<td>1.02</td>
</tr>
<tr>
<td>Total N, g/kg</td>
<td>0.16</td>
<td>0.17</td>
<td>5</td>
<td>0.12</td>
<td>0.17</td>
<td>1.06</td>
</tr>
<tr>
<td>POM-N, g/kg</td>
<td>0.51</td>
<td>0.040</td>
<td>10</td>
<td>0.49</td>
<td>0.042</td>
<td>1.53</td>
</tr>
</tbody>
</table>

Although many others have reported good estimates of soil C with VNIR spectroscopy, the poor results in this study may have been due to the relatively small range of variability across the test area (table 1). The standard deviation of measured SOC was 1.2 g/kg, while the RMSE values reported in previous research for soil C estimation have generally been between 2 and 3.5 g/kg (Viscarra Rossel et al., 2006).

Although the accuracy of the VNIR approach was not sufficient to quantify spatio-temporal differences in SQIs in this study, a higher level of accuracy would be expected with a wider range in indicator values, as when comparing management systems as well as spatio-temporal differences. In future work, we will assess the ability of VNIR spectroscopy to quantify soil quality variations across cropping systems on claypan soil landscapes.

**Conclusion**

In this study, SQIs, particularly POM-C and POM-N, showed significant changes three years after management was changed from a soybean-corn cropping system to a soybean-wheat-hay cropping system. Thus, it appeared that the goal of this new system to increase soil quality was successful, although additional monitoring is needed to assess changes over a longer period of time. The improvement in SQIs was spatially structured, with the largest improvement seen in the lower portions of the landscape where soil conditions were more consistently moist, perhaps supporting greater biological activity.

The VNIR reflectance approach was not able to successfully quantify spatio-temporal differences in SQIs. In general, those SQIs varied by only a small amount in this dataset, making estimation by VNIR particularly challenging. However, we believe that VNIR estimates of SQIs should be feasible in datasets with more variation, such as data collected across contrasting management systems or longer after initiation of a new system. We will investigate this in future research.

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References


