

프로브형 가시광-근적외선 센서를 이용한 토양의 탄소량 측정

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Soil Profile Measurement of Carbon Contents using a Probe-type VIS-NIR Spectrophotometer

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Abstract

An in-situ probe-based spectrophotometer has been developed. This system used two spectrometers to measure soil reflectance spectra from 450 nm to 2200 nm. It collects soil electrical conductivity (EC) and insertion force measurements in addition to the optical data.

Six fields in Kansas were mapped with the VIS-NIR (visible-near infrared) probe module and sampled for calibration and validation. Results showed that VIS-NIR correlated well with carbon in all six fields, with RPD (the ratio of standard deviation to root mean square error of prediction) of 1.8 or better, RMSE of 0.14 to 0.22%, and R^2 of 0.69 to 0.89.

From the investigation of carbon variability within the soil profile and by tillage practice, the 0-5 cm depth in a no-till field contained significantly higher levels of carbon than any other locations. Using the selected calibration model with the soil NIR probe data, a soil profile map of estimated carbon was produced, and it was found that estimated carbon values are highly correlated to the lab values.

The array of sensors (VIS-NIR, electrical conductivity, insertion force) used in the probe allowed estimating bulk density, and three of the six fields were satisfactory. The VIS-NIR probe also showed the obtained spectra data were well correlated with nitrogen for all fields with RPD scores of 1.84 or better and coefficient of determination (R^2) of 0.7 or higher.

Keywords : Near infrared, Carbon, Soil sensors, In-situ probe type spectrophotometer, Soil profile measurement

1. INTRODUCTION

The rapid increase of greenhouse gases in the atmosphere is anticipated to have a negative impact on the global environment. Consequently, an international initiative is underway to find ways to slow the rate of increase of atmospheric greenhouse gases. Long-term approaches will involve future technology for advanced engines and power plants. These options will not be viable for several years to come. However, several short-term options are available including both

biological and geological sequestration of carbon.

Soils lost an estimated 78 giga tons of carbon between the 1850s 2000, primarily due to cultivation (Lal, 2009). This loss of soil carbon represents a significant portion of greenhouse gas emissions, and has resulted in the degradation of agricultural soil quality worldwide. Using practices that restore carbon, such as no-till farming, carbon can be sequestered in the soil. Carbon sequestration has the potential to offset fossil fuel emissions by 0.4 to 1.2 giga tons of carbon per year, or 5 to 15% of the global fossil-fuel emissions (Lal, 2004).

The article was submitted for publication on 2009-05-14, reviewed on 2009-09-04, and approved for publication by editorial board of KSAM on 2009-09-21. The authors are Giyoung Kweon, Research and Development Engineer, Eric Lund, President, Chase Maxton, Engineer, Paul Drummond, Engineer, and Kyle Jensen, Engineer, Veris Technologies, Salina, Kansas, USA. Corresponding author: G. Y. Kweon, Research and Development Engineer, Veris Technologies, 601 N. Broadway, Salina, KS 67401, USA; Phone: +1-785-404-1126; Fax: +1-785-825-6983; E-mail: <gkweon@gmail.com>.

The development and practice of soil carbon sequestration has created a need for better measurement techniques to quantify soil organic carbon across a range of scales. Assessments at regional and national scales are critical for global carbon accounting and policy development. On the other hand, assessments at the project and field scale are critical for developing and evaluating management practices that sequester carbon reliably and economically. Specifically, the researcher may desire to know how various soils or locations within a field respond to treatments. Furthermore, since different treatments may impact the carbon balance at specific locations in the soil profile, variation within a profile must be quantified. While soil maps and soil databases can be effectively used for national carbon inventories, they are not adequate to account for variation and stratification within a single field or research plot (Brown, 2003) and they do not account for changes over time. On the other hand, laboratory methods of measuring soil carbon such as thermal combustion (Nelson and Sommers, 1996) are highly accurate but are labor intensive and expensive.

Thus it is necessary to characterize within field variability with inexpensive and reliable ways. Reflectance spectroscopy is a promising, nondestructive technique for rapid analysis of soil physical and chemical properties to fulfill these requirements.

Numerous laboratory studies have demonstrated the effectiveness of NIR in performing quantitative analysis of soils, including soil C (Hao and Kravchenko, 2007; La et al, 2008; Lee et al., 2008; Reeves et al., 1999; Viscarra Rossel et al., 2005). In addition, several researchers have proposed and tested spectrophotometers for on-the-go in-situ reflectance measurements (Christy et al., 2003; Christy, 2008; Shibusawa et al., 1999; Shonk et al., 1991; Sudduth and Hummel, 1993).



Fig. 1 Field measurement with a VIS-NIR shank system.

A commercially available on-the-go VIS-NIR shank system for measuring near-surface soil properties across a field has been developed by Veris Technologies, Inc. (Fig. 1). However in order to measure variation of soil profile at specific locations, a probe type spectrophotometer is needed.

The objective of this study was to test a VIS-NIR probe unit and processes that acquire soil spectra and auxiliary sensor data in situ, and evaluate its effectiveness in measuring selected soil profile carbon contents.

2. MATERIALS AND METHODS

A. Field Equipment

A probe unit which collects reflectance data through a window on the side is shown in Fig. 2. The probe is optimized to direct diffusely reflected light into optical fiber, and at the same time, light from the internal halogen lamp is directed in a perpendicular direction through the flat sapphire window to minimize internal reflections.

The probe system uses a CCD array spectrometer (USB4000, Ocean optics, USA) and an InGaAs photodiode-array spectrometer (C9914GB, Hamamatsu, Japan) to collect VIS and NIR measurements (450-2200nm).

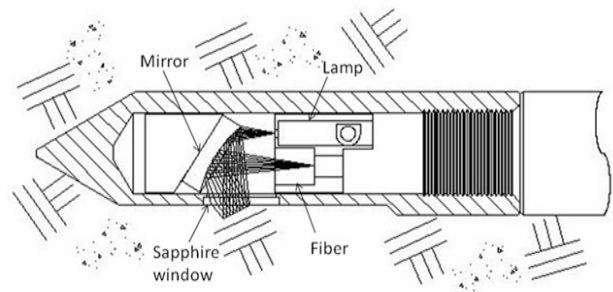


Fig. 2 A cutaway drawing of the soil probe design.

Approximately 20 spectra per second with 8 nm resolution were acquired from the spectrometers and immediately transferred through a universal serial bus (USB) connection to a personal computer for storage. An acquisition program and all subsequent data processing programs were written in Labview (National Instruments, Austin, TX, USA).

At regular intervals during the mapping process, dark and reference measurements are collected by turning off lamp power and placing a known reference material in front of the optic, respectively. The dark measurement is used to

compensate for imperfections in the spectrometer, and the reference measurement is used to compensate for drift in the spectrometer and light source.

The reflectance (R) was calculated using resulting spectrum (I_s), acquired dark (I_d) and reference spectra (I_r), and then converted to absorbance (A) as follows (Christy, 2008):

$$R = \frac{I_s - I_d}{I_r - I_d} \quad (1)$$

$$A = \log_{10} \left(\frac{1}{R} \right) \quad (2)$$

An auxiliary instrument collects GPS data, soil temperature, auxiliary case temperature, auxiliary case humidity, spectrometer case temperature, spectrometer case humidity, and control box temperature. The recorded data is transferred to a personal computer with spectra data for storage. The spectrometer software controls a thermal electric cooler that keeps the temperature of the spectrometer case between 23.4 – 23.9°C.

The probe unit is designed to hydraulically push a probe vertically into the soil profile (Fig. 3(a)) and uses the same spectrometer as a shank NIR system developed by Veris Technologies, Inc. (Fig. 1). It can be attached to a tractor via a 3-point hitch, or can be configured with its own engine and hydraulics and mounted on a truck bed. The hydraulic functions of the probe provide lateral and front-to-back shifting of the probe. This allows repeated insertions in close proximity without moving the vehicle. The rack-and-pinion lateral shifting design keeps the entire probe implement close-coupled to the vehicle. A hydraulic foot assembly provides stability for the probe. The probe is mounted to the implement with a single pin for easy removal, allowing rapid installation of coring probe.

The probe implement also serves as the platform for hydraulically inserting a coring probe into the soil. These soil cores, collected in close proximity to the sensor probe insertions, are lab-analyzed and used to calibrate the sensor measurements to soil properties of interest. The coring probe is constructed of two inch outer diameter steel, and attaches to the probe implement with a coupler and hex-shaped locking collar. For ease of insertion, the core sampler tube may be rotated with a hydraulic motor. The core sampler tube has replaceable cutting shoes that thread onto the tube.

Samples may be collected in polymer liners that insert into the tube, or directly into the steel tube.

The sensor probe is constructed of one inch diameter and 40 inch long hollow-stem probe rod. It has a replaceable conical tip to aid in soil penetration (Fig. 3(b)). Embedded in the conical tip is an EC (electrical conductivity) contact pin, insulated from the probe rod. To measure electrical conductivity, electrical power is injected into the pin, and current and voltage drop are measured at the conical tip. Above the conical tip is a replaceable reflectance module threaded onto the probe rod. At the top of the rod is a load cell that measures the insertion force required to insert the probe. An electronic string potentiometer records the depth during probe insertion. The depth measurements and GPS location are matched with each sensor value at each insertion.



Fig. 3 (a) Soil profile measurement with a probe unit. **Fig. 3** (b) A conical probe tip.

B. Data Acquisition

The spectral and auxiliary data obtained by the probe system is streamed to a file in a compact format. The system requires a dark and reference spectrum about every 10 minutes and no data can be logged if there is no GPS signal or there is a bad reference spectrum.

The VIS-NIR probe module was tested on six Kansas fields, four in Saline county, one in Dickinson county, and one in Ottawa county. Soil types and tillage practice for the fields are shown in Table 1. To investigate carbon variability in soil profiles by tillage practice, both no-till and conventional tilled fields were selected.

On each field, 5-8 locations were identified using either a soil EC or NIR map as having similar soil properties within

Table 1 Study fields location and information

| Field | Soil types | Tillage practice | No. of samples |
|----------|--|------------------|----------------|
| Drummond | Crete silt loam | No-till | 44 |
| Kejr | Detroit silty clay loam, fine sandy loam | No-till | 63 |
| Lund NT | Crete silt loam, Longford silt loam | No-till | 40 |
| Lund CT | Crete silt loam, Longford silt loam | Till | 40 |
| Markley | Crete silt loam, silty clay loam | Till | 50 |
| Tarn | Irwin silty clay loam | No-till | 53 |

a 3-4 m distance. At these stratified locations, three soil profiles were sampled at an equal distance of 3 m, forming a triangle. 0-60 cm profiles were collected using a hydraulic soil sampling probe, and the VIS-NIR/EC/force probe. At each triangle, three 0-60 cm cores were segmented into 0-5, 5-15, 15-30, 30-45, and 45-60 cm segments (Fig. 4).

Soil samples were prepared by drying overnight in a 100°C oven, then grinding to pass through a 2 mm sieve, and analyzed for total organic carbon and total nitrogen on a weight percent basis using a dry combustion method (CN 2000 analyzer, Leco, St. Joseph, MI, USA) in the soil testing laboratory of the Kansa state university. Soil moisture and bulk density was measured on all hydraulic probe core segments receiving carbon analysis in the Veris Technologies' lab.

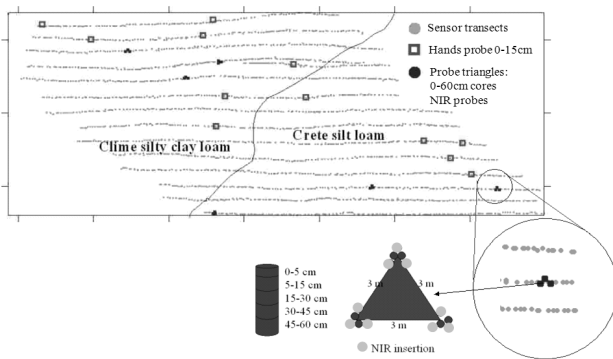


Fig. 4 Example of Kansas field showing mapping and sampling protocols.

C. Data Analysis

1) Interpolation of spectra

In order to create calibrations, the representing spectrum is needed for each recorded soil sample location. An interpolation algorithm can estimate the value at a specific location using the known value at neighboring locations. In this study, a Gaussian weighting method was used (Christy, 2008).

The composite spectrum x_q at the sample point was:

$$x_q = \sum_{i=1}^p w_i x_i \quad (3)$$

where the summation is calculated over the p points, and w is a weight

$$w_i = \frac{e^{-\alpha_i^2}}{\sum_{j=1}^p (e^{-\alpha_j^2})} \quad (4)$$

The weighting parameter, a was measured using

$$\alpha^2 = \left(\frac{\text{longitude}_q - \text{longitude}_i}{a} \right)^2 + \left(\frac{\text{latitude}_q - \text{latitude}_i}{b} \right)^2 + \left(\frac{\text{depth}_q - \text{depth}_i}{c} \right)^2 \quad (5)$$

where q denotes the interpolation location and i denotes a surrounding measurement location.

In this research, 3 m, 3 m, and 0.05 m were used for a , b and c , and the longitude, latitude were converted to meters in the Universal Transverse Mercator (UTM) system.

2) Calibration and validation

The spectra were pretreated using the following pretreatments: spectra only, and spectra with standard normal variate (SNV), 1st Derivative, 1st Derivative & SNV, 2nd Derivative, and 2nd Derivative & SNV. As the pretreatments are being completed, outliers with Mahalanobis distance greater than 3.0 were removed using Eqs. (6) and (7).

$$d_m = \sqrt{(\hat{t}_f - \hat{t})^t C^{-1} (\hat{t}_f - \hat{t})} \quad (6)$$

$$C = \frac{1}{n-1} \hat{T}^T \hat{T} \quad (7)$$

where d_m , Mahalanobis distance, t and T correspond to the vector and matrix respectively of principal component scores and the hat notation is used to indicate that only the first 3 principal component scores are used in the calculation.

The outliers are removed and not used for the calibration. Each target (soil property of interest) is analyzed to remove

outliers that are not within three times the standard deviation from the mean. In addition, each target is transformed using a Box-Cox transform and outliers are calculated in the same way. Whichever method provides the least number of outliers is used for the calibration.

All data is mean centered before partial least square (PLS) regression is used to predict each sampled target value. For every calibration dataset for each field, each pretreatment is applied and a target estimate is calculated, then for each target and pretreatment combination all auxiliary data is individually applied to calculate a target estimate. If any of the auxiliary data improves the calibration, multiple auxiliaries are added to see if there is continued improvement by including more information.

All these possible calibrations are done automatically, and the best calibrations are selected at the end of the program for each field. Once the calibration step has decided which are the best calibrations for every target, that criteria can be applied to the field data to make estimates.

Because calibrations for NIR spectroscopy are empirical in nature, validation is an important part of the process (Christy, 2008). The validation step applies the calibration equation to an independent set of spectra in order to objectively test their performance.

In this study, leave one out cross-validation was used, which leaves one sample out at a time and then uses the other samples to predict the value of the omitted sample. The process is repeated until all samples have been omitted and predicted. A new regression equation is calculated each time that does not include the influence of the left-out sample. Error statistics are based upon the set of predicted values. All programs for calibration and validation were written in Matlab with a PLS toolbox (Eigenvector Research INC., Wenatchee, WA, USA).

3. RESULTS AND DISCUSSION

The results by PLS regression model showed that VIS-NIR correlated well with C in all six fields, with the ratio of standard deviation to RMSECV (RPD) scores of 1.8 or better (Table 2). The pretreatment method selected for the best calibration for each field was also shown in Table 2. For the calibration and validation in this research, the spectra range from 1150 to 2150 nm was selected with 3 latent variables to avoid over fitting. In this test, it was hard to

investigate how tillage practice affects for carbon estimation between no-till fields and tilled fields. The field with the highest RPD and R² is a no-till field (Kejr) and the lowest RPD and R² field is also a no-till field (Drummond). Further researches with multi-fields are required to investigate the effect on the different tillage practice.

Table 2 Cross-validation statistics for carbon contents from VIS-NIR probe

| Carbon (%) | | | | | | |
|------------|----------------------------|------|------|----------------|------|------|
| Field | Pretreatment | Mean | RPD | R ² | RMSE | SD |
| Drummond | Spectra only | 1.27 | 1.81 | 0.69 | 0.22 | 0.4 |
| Kejr | 2 nd derivative | 0.8 | 3.06 | 0.89 | 0.17 | 0.51 |
| Lund_NT | 2 nd Der. & SNV | 1.25 | 2.89 | 0.88 | 0.08 | 0.22 |
| Lund_CT | 2 nd Der. & SNV | 1.13 | 2.09 | 0.77 | 0.20 | 0.42 |
| Markley | 1 st derivative | 0.97 | 2.52 | 0.84 | 0.14 | 0.35 |
| Tarn | 1 st derivative | 1.13 | 1.97 | 0.74 | 0.16 | 0.31 |

Fig. 5 shows carbon variability within the soil profile and by tillage practice. For this test, carbon contents were averaged in the same depths for a no-till field (Lund_NT) and a conventional tilled field (Lund_CT), respectively. Carbon content differences were found within the profile and were in line with expectations for differing tillage practices - a no-till (NT) field had more carbon in the top 15 cm than an adjacent conventionally-tilled (CT) field. The C was stratified by depth, with the 0-5 cm depth in the no-till field containing significantly higher levels of C.

A map of estimated carbon was produced for the soil

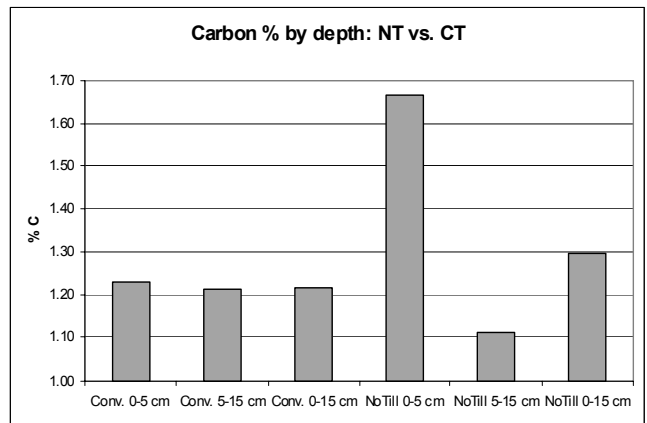


Fig. 5 Carbon contents in top 15 cm in no-till (Lund_NT) and conventionally-tilled (Lund CT) field.

profile from NIR probe calibrations for Kejr field in Fig. 6. The upper figure shows the estimated carbon contents by the PLS calibration with the best model (Table 2), and the lower figure shows the actual lab data used for the calibration. From the figures, it was found that estimated carbon values are highly correlated to the lab values.

Fig. 7 shows soil carbon patterns of a transect that was intensely NIR-profiled along a field. The results demonstrate the ability of NIR probing to depict subsurface carbon variability, and detect spatially-structured and elevation-related soil carbon patterns.

The array of sensors used in the probe, VIS-NIR, EC, and force, are typically related to soil moisture, texture, and soil strength. As a result, this combination of measurements may be able to estimate bulk density, a factor extremely important in measuring carbon change. Estimations of bulk density on three of the six fields were satisfactory (Table 3). In this test, mostly conventional tilled fields showed better results for RPD and R^2 than no-till fields.

The in-situ probe-based VIS-NIR spectrophotometer also showed the spectra data were well correlated with nitrogen for six Kansas fields with RPD scores of 1.84 or better and

R^2 of 0.7 or higher in Table 4. The result showed very similar to the carbon contents estimation (Table 2). Kejr field showed the highest RPD and R^2 and Drummond field showed the lowest RPD and R^2 . However it was hard to find a tillage effect on nitrogen estimation between no-till fields and tilled fields, therefore more researches are necessary.

Fig. 8 shows the relationship between carbon contents and nitrogen contents for all the 6 KS fields' data, and they are highly correlated to each other. Nitrogen contents may be helpful to estimate carbon contents with other auxiliary data such as EC.

Table 3 Cross-validation statistics for bulk density from VIS-NIR probe

| Bulk density (g/cm ³) | | | | | | |
|-----------------------------------|------------------------------------|------|------|-------|------|------|
| Field | Pretreatment | Mean | RPD | R^2 | RMSE | SD |
| Drummond | Spectra only | 1.61 | 1.11 | 0.21 | 0.12 | 0.14 |
| Kejr | Spectra & SNV & force | 1.78 | 1.28 | 0.40 | 0.13 | 0.17 |
| Lund_NT | 1 st Der. & SNV | 1.7 | 2.09 | 0.76 | 0.07 | 0.14 |
| Lund_CT | 1 st Der. & SNV & force | 1.71 | 2.16 | 0.78 | 0.08 | 0.18 |
| Markley | SNV & force | 1.54 | 1.95 | 0.73 | 0.10 | 0.19 |
| Tarn | SNV | 1.58 | 1.59 | 0.61 | 0.11 | 0.17 |

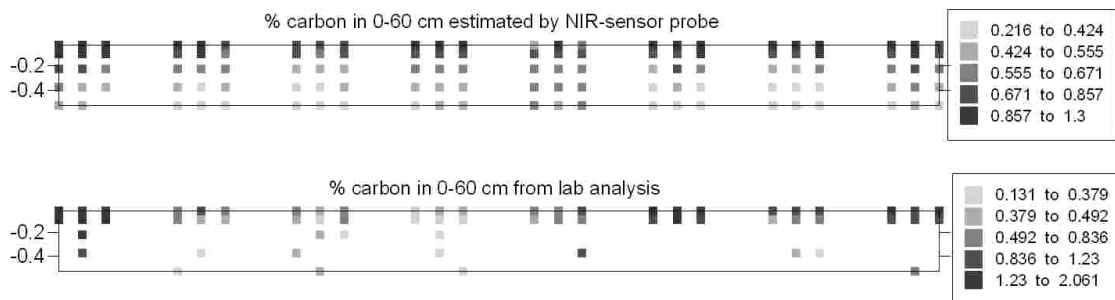


Fig. 6 Kejr field with all probe samples and sensor data calibrated to lab-analyzed C.

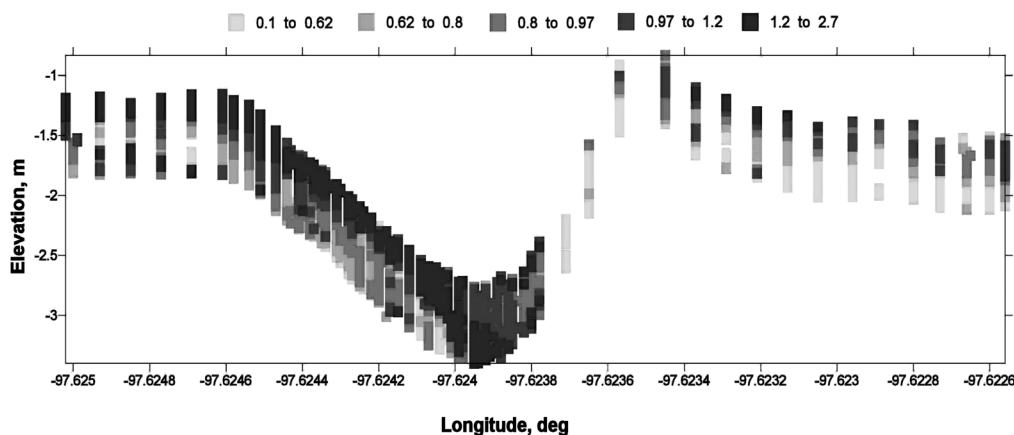


Fig. 7 Elevation-related soil carbon patterns along transect in the field.

Table 4 Cross-validation statistics for Nitrogen contents (%) from VIS-NIR probe

| Nitrogen (%) | | | | | | |
|--------------|----------------------------|------|------|----------------|------|------|
| Field | Pretreatment | Mean | RPD | R ² | RMSE | SD |
| Drummond | 1 nd Der. & SNV | 0.12 | 1.84 | 0.70 | 0.02 | 0.03 |
| Kejr | 2 nd derivative | 0.08 | 3.39 | 0.91 | 0.01 | 0.04 |
| Lund_NT | 2 nd Der. & SNV | 0.13 | 2.09 | 0.77 | 0.20 | 0.42 |
| Lund_CT | 2 nd Der. & SNV | 0.12 | 2.75 | 0.87 | 0.01 | 0.02 |
| Markley | 2 nd Der. & SNV | 0.09 | 2.17 | 0.78 | 0.01 | 0.03 |
| Tarn | 2 nd Der. & SNV | 0.1 | 2.38 | 0.82 | 0.01 | 0.03 |

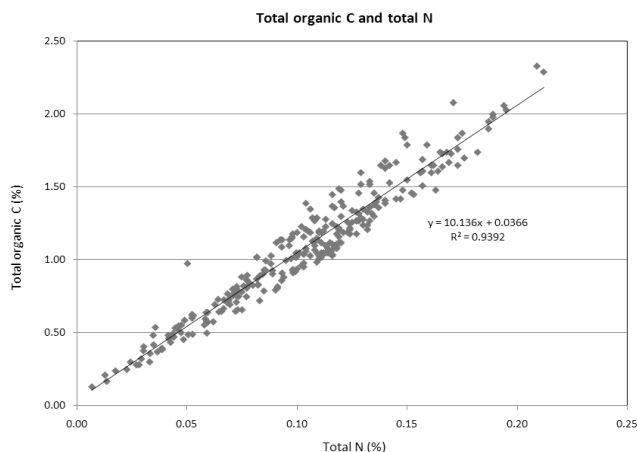


Fig. 8 Plot of total organic C and total N for 6 KS fields.

4. CONCLUSIONS

An in-situ probe-based spectrophotometer has been developed. This system used two spectrometers to measure soil reflectance spectra from 450 nm to 2200 nm, and also collects soil electrical conductivity and insertion force measurements.

The objective of collecting VIS-NIR data in situ with a field-deployed spectrometer probe, and evaluating the effectiveness in measuring selected soil profile carbon and other properties was successfully attained. Major findings were:

- (1) Usage of the Mahalanobis distance metric allowed samples to be screened before the application of the calibration. Samples that did not sufficiently match the calibration set were not predicted.
- (2) PLS regression was used to develop calibration, and using leave one out validation, which matches the prediction problem posed by real-time measurements, the system predicted carbon with RMSE of 0.14 to 0.22% and R² of 0.69 to 0.89 for six Kansas fields between the laboratory measurements and probe VIS-

NIR system predictions.

- (3) From the investigation of carbon variability within the soil profile and by tillage practice, carbon content differences were found within the profile and the 0-5 cm depth in a no-till field contained significantly higher levels of C than any other locations. Using the best calibration model with the soil NIR probe data, a map of estimated carbon was produced, and it was found that estimated carbon values are highly correlated to the lab values.
- (4) The array of sensors used in the probe—VIS-NIR, EC, and force, are typically related to soil moisture, texture, and soil strength. As a result, this combination of measurements may be able to estimate bulk density. In this study, however, three of the six fields were satisfactory for the estimations of bulk density. Further investigation of data calibration and validation, uses of various types of sensors and multi-fields researches are needed to improve the estimations of bulk density.
- (5) The in-situ probe-based VIS-NIR spectrophotometer also showed the spectra data were well correlated with nitrogen for six Kansas fields with RPD scores of 1.84 or better and R² of 0.7 or higher.

Acknowledgement

Funding for NIRS research was provided by the Small Business Innovation Research programs of the U.S. Departments of Agriculture and Energy.

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