Spectral reflectance measurements for organic matter sensing in Saskatchewan soils

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Ingleby, H.R. and Crowe, T.G. 1999. **Spectral reflectance measurements for organic matter sensing in Saskatchewan soils.** Can. Agric. Eng. **41**:073-079. Diffuse reflectance spectra from 250 to 2500 nm were measured for soil samples taken from five Saskatchewan fields. The five fields represented a range of organic carbon levels varying between 0.55 and 5.34%. The efficacy of two previously published equations relating reflectance values at specific wavelengths to the soil organic carbon content was evaluated using these data. While one method resulted in a coefficient of determination (r^2) greater than 0.8 for all samples, neither method was suitable for implementation in a soil organic matter sensor. Further investigation into methods for determining an optimum wavelength set for organic carbon prediction in Saskatchewan soils is recommended.

Le spectre de réflexion diffuse pour des longueurs d'onde variant entre 250 et 2500 nm a été mesuré sur des échantillons de sol provenant de 5 champs de la Saskatchewan durant le mois de mai. Les échantillons avaient des niveaux de carbone variant entre 0.55 et 5.34%. L'efficacité de 2 équations publiées précédemment et reliant les valeurs de réflectance à des longueurs d'onde spécifiques avec le % de carbone contenu dans le sol a été évaluée avec ces données. Bien qu'une des équations utilisées donne des coefficients de détermination (r^2) supérieurs à 0.8 pour tous les échantillons, aucune des 2 méthodes ne s'est révélée adéquate pour être utilisée dans la fabrication d'un appareil servant à mesurer le taux de carbone dans les sols organiques. D'autres recherches devront donc être effectuées de façon à déterminer les longueurs d'onde optimales pour la reconnaissance du taux de carbone dans les sols organiques de la Saskatchewan.

INTRODUCTION

Site-specific crop management (SSCM) practices, including prescription application of fertilizers and herbicides, have the potential to provide significant savings over traditional uniform-coverage methods. Implementation of SSCM practices requires that producers are aware of within-field variations in soil properties. An important variable in soil management is the organic matter content of the soil. Adsorption of soil-applied herbicides by soil organic matter (SOM) can reduce the amount of chemical that is available for weed control. Thus, the ability to sense varying levels of SOM is necessary when trying to simultaneously minimise chemical use and ensure efficacy in weed control. Because the organic matter content can vary significantly within a field, automatic adjustments to the rate of herbicide application require sensors capable of rapidly determining the amount of organic matter present in the soil.

Organic matter is usually defined as the total amount of nonliving organic carbon-containing substances in the soil (Senesi and Loffredo 1998). The organic matter content of soil is typically determined by measuring the amount of organic carbon (OC) present. The organic matter content, expressed on a percent dry-mass basis, is equal to 1.72 times the organic carbon content in percent (Krishnan et al. 1980). The terms OM and OC are generally used interchangeably, yet are not identical in meaning.

Soils with high organic carbon contents are typically darker than those with lower levels. Variations in soil color can be quantified using spectral reflectance measurements in the visible portion of the spectrum. Reflectance in other wavebands may also be correlated with the presence of organic carbon. Spectral reflectance may provide a means of realising a rapid, non-contact, soil organic carbon sensor.

The influence of soil characteristics other than organic carbon content on reflectance must be considered when attempting to identify possible correlations, because soil parent material, structure, and chemical composition may vary widely from field to field. A reflectance-based soil organic carbon sensor, applicable to a wide range of soils, is not currently commercially available. Before such a sensor can be realised, a better understanding of the range of soil organic carbon levels and associated spectral characteristics over a wide geographical area is required.

LITERATURE REVIEW

The spectral reflectance of soils has been investigated by a number of researchers and the influence of various soil characteristics such as parent material, organic matter, iron oxides, and mineral content on reflectance has been documented. A sample of researchers reporting these data includes Obukhov and Orlov (1964), Bowers and Hanks (1965), Stoner and Baumgardner (1981), and Baumgardner et al. (1985).

A number of studies have sought specific correlations between soil organic carbon levels and reflectance spectra. Krishnan et al. (1981) used stepwise multiple linear regression to identify optimum predictor wavelengths for a data set of 10 Illinois soils. Before the regression was performed, raw reflectance spectra were transformed into optical density (OD) values (OD = log (1/R), where R = fractional reflectance value). The regression model was based on the ratio of the first derivative of the OD value at two wavelengths, 623.6 and 564.4 nm. This resulted in a coefficient of determination (r^2) of 0.92. Similarly, Smith et al. (1987) generated several linear regression models using 30 representative Illinois soils. Models, which incorporated ratios of OD values for 4 and 8

Table I. Locations and descriptions of sampled fields in Saskatchewan.

Field	Soil zone	Soil association	Soil texture	Location*
Hepburn	Black	Oxbow	loam	SE-7-40-5-W3
Outlook	Dark Brown	Elstow	loam	SE-20-28-7-W3
Swift Current	Brown	Haverhill	loam - sandy loam	NE-22-15-12-W3
Watrous	Dark Brown	Weyburn	loam	NW-13-32-26-W2
St. Louis	Black	Hamlin - Blaine Lake	fine sandy loam - silty loam	SE-20-46-26-W2

* Quarter-Section-Township-Range-Central Meridian

wavelengths, resulted in r^2 values of 0.80 and 0.86, respectively. Subsequently, Sudduth and Hummel (1991) performed validation tests on these equations and showed better performance with the 4 - wavelength model, perhaps due to overfitting to the calibration data with the 8 - wavelength model. Dalal and Henry (1986) also used the OD transformation and generated a predictive equation using three wavelengths (1744, 1870, and 2052 nm) which resulted in r^2 values greater than 0.8 for three series of Australian soils.

In addition to confirming work by Smith et al. (1987), Sudduth and Hummel (1991) examined several methods for generating organic carbon calibration equations based on reflectance data. They obtained very good predictive performance (r^2 = 0.91) using a partial least squares (PLS) regression on NIR reflectance values transformed to OD values. Sudduth and Hummel (1993a, 1993b) later developed a portable NIR spectrophotometer with predictive ability approaching that of a laboratory instrument (r^2 = 0.89) using prepared samples. The developed instrument was less successful in field tests and extension of this testing to a wider geographical range (Sudduth and Hummel 1996) resulted in a further reduction in predictive accuracy.

OBJECTIVES

The previously identified research was completed primarily in the United States. Given that researchers have shown localized differences in soil spectral characteristics, it is not clear whether previously defined prediction models can be successfully implemented in Western Canada. In this study, the use of soil reflectance was investigated as a potential mechanism for detecting soil organic carbon. The objectives of this study were to:

1) document the range of spectral reflectance characteristics and associated organic carbon content in five Saskatchewan fields and
2) determine the efficacy of soil organic carbon predictors developed by other researchers when applied to these spectra.

MATERIALS and METHODS

Sample collection and preparation

Four hundred twenty soil samples were collected from five Saskatchewan fields in May of 1997. The fields were identified by the nearest urban center, so that the five fields were labeled as Hepburn, Outlook, Swift Current, Watrous, and St. Louis. Ninety samples were collected from each of the first four fields and sixty samples from the fifth field. Table I consists of a list of the fields, legal locations (quarter section, township and range), and the soil descriptions. The five fields were distributed across three soil zones in Saskatchewan (Black, Dark Brown, and Brown). Soil samples were collected from each field such that three slope positions were defined in the first four fields and two were sampled in the fifth field. The same number (30) of samples was collected from the lower, mid, and upper slopes of four of the fields, while samples from the fifth field were collected from the lower and upper slope regions only. The soil cores were taken from each slope position to a 150 mm depth within the Ap horizon for each field. The samples were air-dried for a minimum of 15 h at 32 °C, ground, and passed through a 2-mm mesh sieve. Obvious organic debris was removed prior to grinding.

Soil property measurement

Diffuse reflectance spectra were obtained with a UV-Vis-NIR spectrophotometer (Cary 5G, Varian Canada Inc., Mississauga, ON) equipped with a 110-mm diameter integrating sphere. Averaged triplicate reflectance values were recorded at one-nanometer (nm) increments from 250 to 2500 nm for each of five sub-samples. Each of the soil samples was separated into five sub-samples. Thus, 2100 scans were completed by the spectrophotometer. An average reflectance spectrum for each soil sample was determined off line by calculating the mean reflectance from the five sub-samples. Reflectance values were recorded as percentages, with 100 percent representing an ideal diffuse reflector, relative to a baseline obtained with a polytetrafluoroethylene (PTFE) reference standard.

Total organic carbon content was determined for each soil sample by combustion of a portion of each sample at 840 °C (Leco CR-12 Carbon Determinator, Leco Corp., St. Joseph, MI). This temperature allowed for combustion of organic-C components only, leaving inorganic-C components intact. The level of organic carbon was expressed as a percentage of the air-dried mass.

Data analysis

Multiple examples of predictors for soil organic carbon based on reflectance data are represented in the literature. Two such examples were presented by Dalal and Henry (1986) and Smith et al. (1987), subsequently referred to in this paper as method 1 and method 2, respectively. These methods were selected for testing with the Saskatchewan field data based on the quality of fit achieved with their original data sets. Each method performed well with the original data and resulted in coefficients of determination (r^2) greater than 0.8. Both methods used an optical density transformation of raw reflectance values. Method 1 used a multiple linear regression of the form:

$$OC = a_0 + a_1 OD_{1744} + a_2 OD_{1870} + a_3 OD_{2052} \quad (1)$$

where:
OC = organic carbon content (%),
a_0, a_1, a_2, a_3 = regression coefficients, and
OD_n = optical density at wavelength n (nm).

Method 2 used a simple linear regression of the form:

$$OC = k_0 + k_1 \left[\frac{OD_{424.0} - OD_{808.0}}{OD_{575.2} - OD_{548.8}} \right]^{*} \quad (2)$$

where: k_0, k_1 = regression coefficients.
*Because data in this study were recorded at 1-nm intervals, fractional wavelengths in Eq. 2 were taken to the nearest nm.

Regression coefficients were determined for each method on a field-by-field basis and for all five fields as an aggregate. The adequacy of each fitted regression model was determined by calculating a coefficient of determination (r^2) value (Walpole and Myers 1989).

RESULTS and DISCUSSION

Soil reflectance data

Mean reflectance curves for Hepburn, Outlook, Swift Current, Watrous and St. Louis fields are given in Fig. 1. Minimum and maximum reflectance curves, along with the mean reflectance curves, are shown in Figs. 2 through 6 for the fields individually. These minimum and maximum curves show the lowest and highest reflectance values at each wavelength across all samples for each field. The minimum and maximum curves provide an indication of the variation in spectral reflectance between samples from the same field.

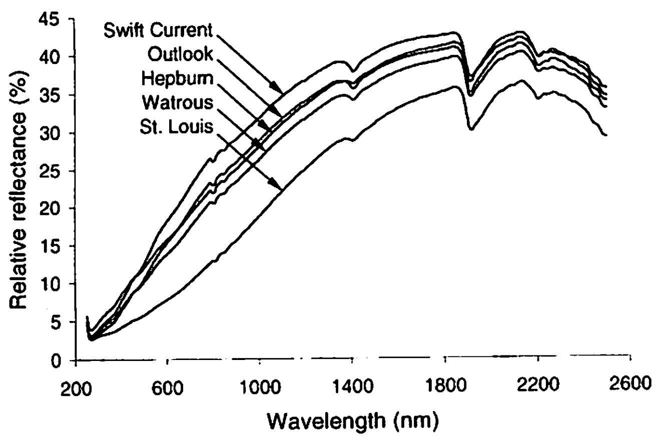

Fig. 1. Mean reflectance spectra for all fields.

The mean reflectance curves (Fig. 1) illustrate the field-to-field differences in spectral reflectance with peak reflectance levels being approximately 40%. The soil samples had little reflectance in the UV range and reflectance gradually increased through the visible wavelengths. In the near infrared region, reflectance values were relatively high and gradually decreased beyond 2100 nm. Noticeable absorption bands were present at 1450, 1950, and 2200 nm. According to Baumgardner et al. (1985), the first two bands were due to water absorption and the last is a result of a vibrational mode of the hydroxyl ion.

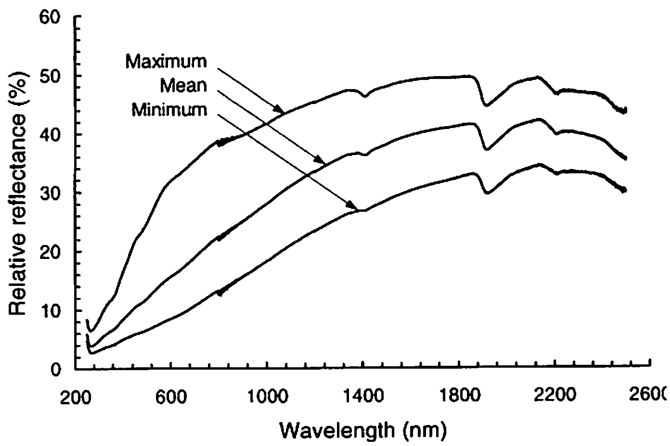

Fig. 2. Mean, minimum, and maximum reflectance spectra for Hepburn field.

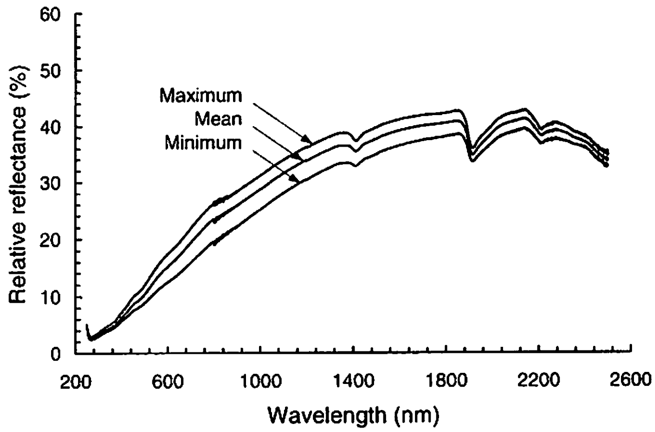

Fig. 3. Mean, minimum, and maximum reflectance spectra for Outlook field.

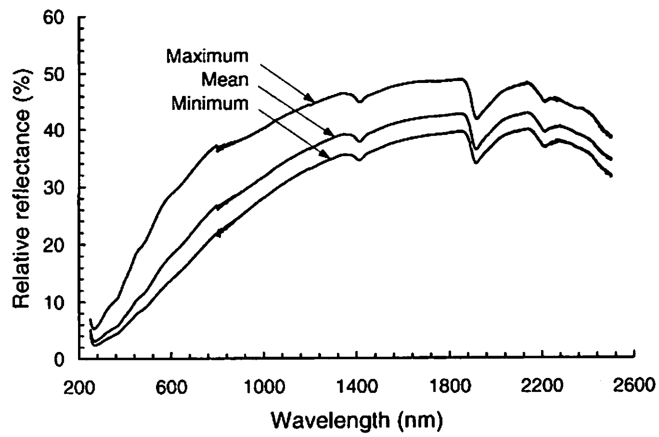

Fig. 4. Mean, minimum, and maximum reflectance spectra for Swift Current field.

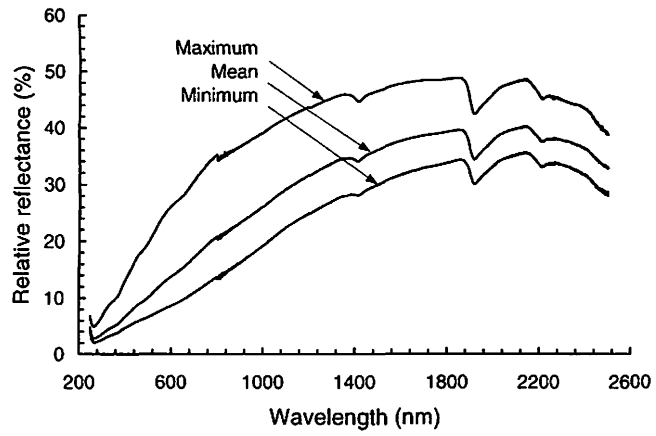

Fig. 5. Mean, minimum, and maximum reflectance spectra for Watrous field.

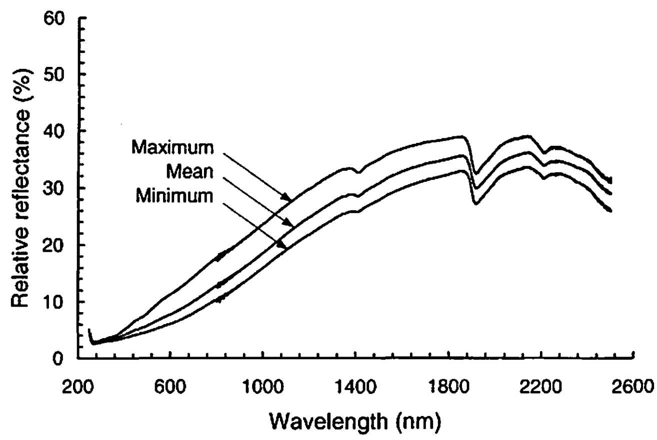

Fig. 6. Mean, minimum, and maximum reflectance spectra for St. Louis field.

Table II. Organic carbon levels for each field individually and as an aggregate determined by combustion of soil samples.

Field	Mean OC (%)	Minimum OC (%)	Maximum OC (%)
Swift Current	1.22	0.55	1.81
Outlook	1.62	1.26	2.19
Hepburn	2.21	0.87	3.23
Watrous	2.39	0.78	4.04
St. Louis	3.38	1.30	5.34
Aggregate	2.08	0.55	5.34

Baumgardner et al. (1985) also indicated that the mineral composition of a soil, the presence of iron oxides, and the parent material from which a soil was formed would influence its reflectance characteristics. In all of the reflectance spectra, there was an erratic noise-like feature near 800 nm. This

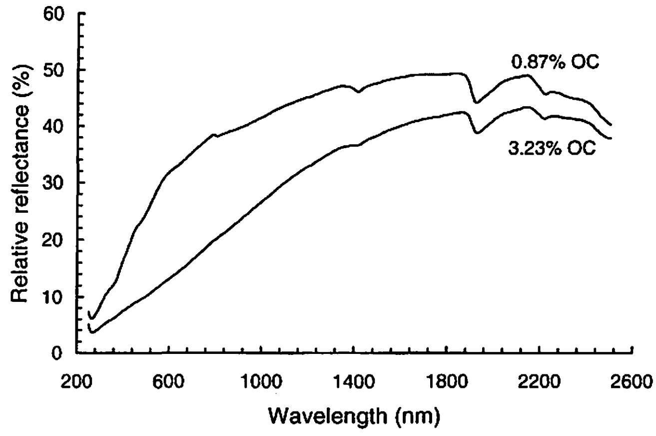

Fig. 7. Spectra for high and low OC content samples from Hepburn field.

variability was due to detector changeover during spectrophotometer operation.

Mean, minimum, and maximum OC levels for each field and for all five fields as an aggregate are given in Table II. The sequence of fields arrayed by mean OC content shows that the St. Louis field had the highest mean OC level (3.38 %), and the Swift Current field the lowest (1.22 %). This sequence equalled the reverse of that obtained in spectral reflectance (Fig. 1). Generally, the St. Louis field (Fig. 1) had soil with the lowest reflectance, while the Swift Current field (Fig. 1) had soil with the highest reflectance.

Figures 2 to 6 show that the range of spectra was substantial in the Watrous and Hepburn fields and to a lesser degree in the Swift Current field. Reflectance variations between samples were small in the Outlook and St. Louis fields. Color differences between samples from the same field were also apparent. Visual inspection of the samples showed soil colors ranging from a light tan to a dark brown. Note that human color perception is based on sensing reflectance in the 400 to 760-nm waveband. Samples from the Outlook field showed the greatest color homogeneity. This is expected given the small differences between spectra in Fig. 3. Comparison of Figs. 2 to 5 with data given in Table II displayed a correspondence between within-field spectra variations and the range of OC content. For these four fields, a large difference between the minimum and maximum reflectance curves was associated with large variability in OC levels within the field. This relationship was not present in the St. Louis spectra (Fig. 6). This suggests that a wide range of OC levels may not always translate into large differences in reflectance spectra.

Spectra for two samples with high and low OC levels from the Hepburn field are given in Fig. 7. Inspection of the reflectance curves for samples with different OC levels showed differences in the relative reflectance values. However, no distinct absorption bands corresponding to changing OC levels appeared to be present. Wavelengths at which the reflectance was strongly correlated with the soil's OC content were not immediately apparent and will require further investigation.

Prediction models

Coefficients of determination for the regression methods tested were calculated for all five fields individually and as an aggregate (Table III). They show that the quality of fit achieved with method 1 was markedly superior to that for method 2. The performance of method 1 was reasonable for the fields individually and was quite good when all soil samples were treated as an aggregate. Use of method 2 resulted in low coefficients of determination for four of the fields and for the aggregate and almost no correlation with the Swift Current field data. Regression coefficients for both methods are given in Table IV.

Table III. Coefficients of determination for methods 1 and 2 (Eqs. 1 and 2).

Field	Method 1	Method 2
Hepburn	0.77	0.52
Outlook	0.62	0.43
Swift Current	0.62	0.03
Watrous	0.75	0.57
St. Louis	0.82	0.19
Aggregate	0.81	0.35

Plots of predicted versus measured OC content for the aggregate of all five fields are given in Figs. 8 and 9 for methods 1 and 2, respectively. The 45° line indicates perfect correlation between predicted and measured values ($r^2 = 1.00$). Figures 8 and 9 show that the predictive ability of both methods was poor at relatively high OC levels. The performance of method 1 (Fig. 8) was questionable beyond 4.0% OC, while method 2 (Fig. 9) performed best below 3.0% OC. Performance of a given predictor would seem to depend both on the wavelengths selected as dependent regression variables and on the form of the equation. Method 1 provided much better results than method 2. Performance with method 1 was still inconsistent between fields and would require improvement before being implemented in a working soil OC sensor.

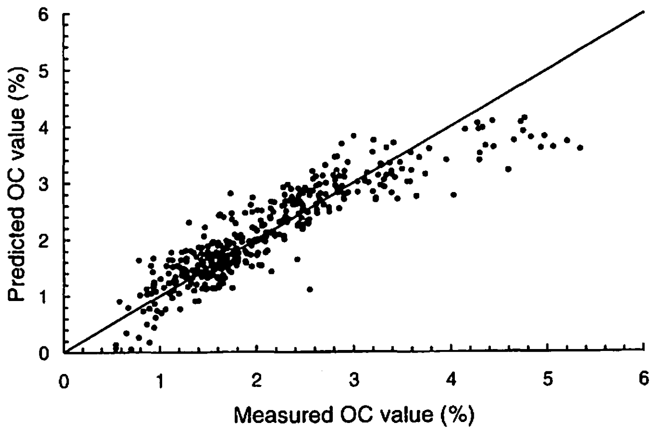

Fig. 8. Predicted versus measured OC content for method 1.

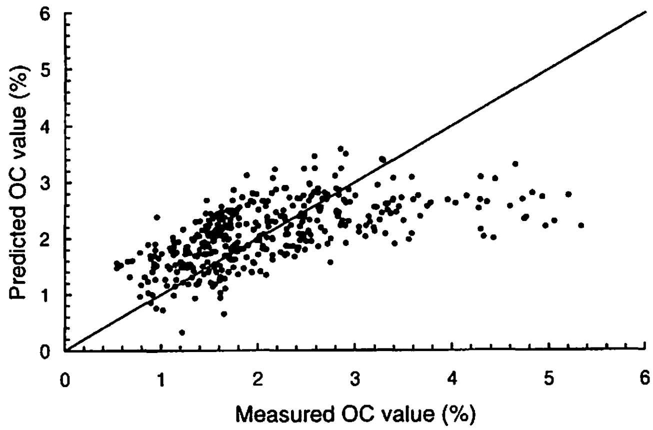

Fig. 9. Predicted versus measured OC content for method 2.

Table IV. Regression coefficients for methods 1 and 2 (Eqs. 1 and 2).

Field	Method 1				Method 2	
	a_0	a_1	a_2	a_3	k_0	k_1
Hepburn	2.81	195.95	-250.05	49.96	-4.19	-0.48
Outlook	-0.93	73.01	-69.11	2.25	-2.91	-0.35
Swift Current	2.16	93.97	-70.93	-24.71	-0.39	-0.13
Watrous	3.47	165.85	-159.58	-10.91	-7.96	-0.80
St. Louis	7.35	350.27	-343.55	-22.02	-7.53	-0.82
Aggregate	1.99	232.80	-301.38	66.57	-7.96	-0.77

Increasing OC levels in soils are usually associated with decreases in the reflectance values across a wide range of wavelengths. Decreasing reflectance values equate to increasing OD values after transformation. Thus, soils with higher OC contents are expected to have higher OD values than soils with lower OC. The regression coefficients in Table IV for method 1 have both strong positive and strong negative values. This indicates that the proportionality between higher OC and higher OD values that is expected may not hold for all wavelengths. Method 2 uses a ratio of OD values at various wavelengths, which may increase or decrease with increasing OC depending on the relative magnitudes of the OD values. Further investigation of the relationships between changing OC levels and the resulting changes in reflectance (or optical density) at various wavelengths is required to determine an optimum wavelength subset for regression model development.

The reflectance wavelengths used in method 1 were all in the NIR region, while those in method 2 were primarily from the visible portion of the spectrum. Thus, it might be concluded that NIR wavelengths provide superior predictive ability for soil OC levels, if the form of the equation is not considered. However, because the color variation between soils with different OC levels has been well documented, it would be prudent to continue investigations with visible wavelengths. Improvements in predictor performance should be possible through identification of the optimum wavelengths and possibly through alternative data transformation and regression methods.

CONCLUSIONS

Reflectance spectra for soil samples across three Prairie soil zones and different organic carbon levels from Saskatchewan fields exhibit significant differences. The greatest variation in within-field spectra was present in the Hepburn field, where the range of OC levels was 0.87 to 3.23%.

The performance of two previously published OC predictive models based on reflectance values varied considerably. Method 1 incorporated NIR reflectance data and was superior to method 2, but would not be adequate for implementation in an OC level sensor.

Methods for selection of an optimum wavelength set for these data should be investigated along with various techniques for applying reflectance values at these wavelengths in an effective predictive model. Such an investigation should include methods such as PCA, PLS, and/or neural networks.

RECOMMENDATIONS

The success of a multiple linear regression (MLR) model depends primarily on the wavelengths selected as the independent regression variables and these wavelengths will be dictated by the data set. Specific wavelengths for the Saskatchewan soils must be evaluated and selected by some iterative process that provides a measure of the ability of the reflectance at each wavelength to discriminate between samples. Algorithms for wavelength selection are discussed in the literature (Hruschka 1987) and should be considered in future work.

Model development using data transformation methods has also been widely applied to spectral discrimination problems. Techniques such as Principal Component Analysis (PCA) and Partial Least Squares (PLS) regression involve the application of a linear transformation to the data set. Both methods have been used in a variety of spectral discrimination and chemometrics applications (Sudduth and Hummel 1991; Ehsani et al. 1997) and should be considered as alternatives to MLR for use with reflectance data.

Methods other than regression are also available once the optimum wavelength set has been determined. Pattern recognition techniques, which construct a decision function based on the chosen features, can be implemented to segregate soils into separate classes based on OC content. Use of a neural network to predict the OC levels of new samples based on the reflectance values at various wavelengths is also possible. In addition to PCA and PLS, non-linear predictive models should also be investigated.

Soil samples in this study were carefully prepared in a laboratory setting before reflectance measurements occurred. To develop a robust sensor for in situ analysis, the effects of varying levels of moisture, soil nutrients, and foreign matter on soil reflectance must be investigated. The predictive model implemented in the sensor should accommodate variations in field conditions without seriously compromising accuracy.

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