

The potential of near infrared reflectance spectroscopy as a tool for spatial mapping of soil composition for use in precision agriculture

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Introduction

Implementation of site-specific (precision) agriculture requires generation of extensive Geographic Information System (GIS) data layers containing information on soil properties, and conventional laboratory analyses for soil are too costly and labour intensive for generating the necessary data.^{1,2} Work by others,^{3,4} and preliminary studies on soils obtained from field studies on the effects of tillage, fertilisation and depth on soil parameters, such as organic C, total N, pH and various forms of biologically-active N showed that near infrared (NIR) reflectance spectroscopy holds promise as a rapid analytical tool for producing estimates of multiple soil properties through a single routine analysis.⁵ However, the 179 samples studied were obtained from plots where the type of soil was generally the same, as this was not a design parameter of the study. In order to utilise NIR for precision agriculture over large areas, calibrations will have to handle variations in soil type. The objective of this work was to investigate the potential of NIR under conditions where variations in the inorganic constituents of the soil were present.

Materials and methods

Two sets of samples were collected from a 20 ha agricultural field which comprised a substantial part of a toposequence within a small watershed. The first consisted of 64 samples randomly collected across the 20 ha field. This set was used for initial assessment of the feasibility of using NIR for mapping soil properties within a toposequence. The second set consisted of 547 samples (one sample lost) collected in a grid pattern from the surface and from a depth of 20 cm at 274 locations.

Samples were scanned from 400 to 2498 nm on a Foss-NIRSystems model 6500 scanning monochromator (Foss-NIRSystems, Silver Spring, MD, USA) equipped with a rotating sample cup. The set of 64 samples was scanned as is and then ground in a Tekmar A-10 Analytical grinder (Tekmar-Dohrmann, Cincinnati, OH, USA). The set of 547 samples were ground by hand using a mortar and pestle. All samples were analysed for total C and N by combustion, using a Leco CNS-2000 Elemental Analyser (Leco Corp., St Joseph, MI, USA).

Calibrations were developed using partial least squares (PLS) regression and a one-out cross-validation (unless otherwise noted) running under GRAMS/386 PLSplus V2.1G (Galactic Industries Corporation, Salem, NH, USA).

Table 1. Carbon and nitrogen contents (% dry matter) of soil samples and correlation between carbon and nitrogen.

Set ^b	<i>n</i>	Carbon				Nitrogen				$C \times N^a$ <i>r</i>
		Mean	<i>SD</i> ^c	Min. ^d	Max. ^e	Mean	<i>SD</i>	Min.	Max.	
1	64	1.60	0.44	0.53	2.80	0.14	0.04	0.05	0.22	0.970
2	547	1.20	0.55	0.37	3.28	0.10	0.05	0.01	0.26	0.966
3	523	1.17	0.52	0.37	3.28	0.10	0.04	0.02	0.23	0.973
4	509	1.16	0.51	0.37	2.71	0.10	0.04	0.02	0.23	0.978
5	179	1.34	0.46	0.61	3.39	0.12	0.04	0.06	0.28	0.989

^a Correlation between C and N contents

^b Set 1 = 64 samples randomly collected (see methods), Set 2 = 547 samples collected using a grid from same field as set of 64, Set 3 = 523 samples remaining after removal of 24 outliers from set of 547, Set 4 = 509 samples after further removal of 14 outliers from set of 523, and Set 5 = 179 samples from previous study

^c Standard deviation of the mean

^d Minimum

^e Maximum

Results and discussion

The data in Table 1 shows the composition of various subsets of samples used in this study. As can be seen, while there were differences in the various sets, for the most part, the range of values for C and N were similar among the various sets. The biggest difference in the various sets was between Set 5 from an earlier study⁵ and the four sets of data from this study (Sets 1–4). In the first study, samples were taken from five depths at two sites, (Piedmont region and Delmarva Peninsula) in MD, containing plow-tilled and no-tilled plots, while the new samples for this study were only taken from two depths, and the entire field was tilled prior to planting the previous spring (samples collected in the winter following the growing season). While samples from the first study were diverse in the nature of treatments used, the soils themselves were much less diverse than the new samples used in this study. All samples from both studies were from fields planted in corn. It should also be noted that the correlation between C and N was higher in the first study (Set 5) than for the new sample sets. In the earlier study, PLS results and factors were very similar for C and N indicating that the same constituents were, for the large part, being determined for both C and N or even one being determined in terms of the other. The lower correlations for the new sample sets makes the latter less likely to be as true or possible for these samples. Finally, while samples from the previous study varied little in colour, the soil samples collected within the watershed for this study varied substantially (from yellowish brown to very dark brown).

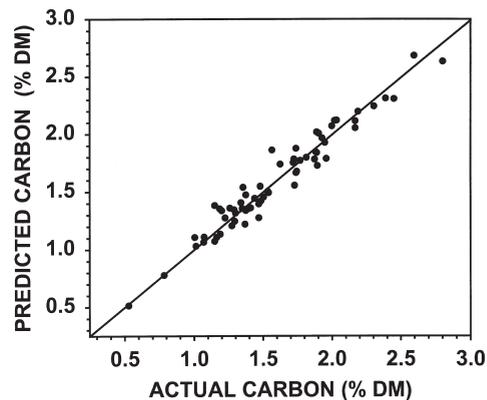


Figure 1. Final calibration results for C resulting from 8-out cross-validation analysis using set of 64 ground soil samples.

Table 2. One-out cross-validation and final calibration results using set of 64 samples.

		Carbon results				
		One-out cross-validation			Calibration results	
Samples/PLS ^a	SpecR ^b	Math-F ^c	R ²	RMSD ^d	R ²	RMSD
Ground/1-out	NIR	2 nd /4-5	0.850	0.169	0.926	0.118
Ground/8-out	NIR	2 nd /4-6	0.843	0.173	0.947	0.101
Ground/16-out	NIR	2 nd /4-3	0.827	0.182	0.853	0.168
Ground/1-out	SW+NIR	2 nd /16-4	0.820	0.186	0.873	0.156
Unground/1-out	NIR	2 nd /4-5	0.718	0.232	0.782	0.204
Unground/8-out	NIR	2 nd /4-5	0.689	0.244	0.782	0.204

		Nitrogen results				
		One-out cross-validation			Calibration results	
Samples/PLS ^{a1}	SpecR ^b	Math-F ^c	R ²	RMSD ^d	R ²	RMSD
Ground/1-out	NIR	2 nd /4-5	0.771	0.0168	0.892	0.0115
Ground/8-out	NIR	2 nd /4-6	0.774	0.0167	0.922	0.0098
Ground/16-out	NIR	2 nd /4-3	0.736	0.0180	0.770	0.0168
Ground/1-out	SW+NIR	2 nd /32-3	0.723	0.0185	0.760	0.0172
Unground/1-out	NIR	2 nd /4-5	0.681	0.0198	0.749	0.0180
Unground/8-out	NIR	2 nd /4-5	0.671	0.0200	0.749	0.0180

^aState of samples / number of samples left out in cross-validation

^bNIR = 1100 to 2498 nm, SW + NIR = 400 to 2498 nm

^cDerivative / derivative gap—number of factors used

^dRoot mean squared deviation

PLS regression results, using the set of 64 randomly collected samples, are presented in Table 2. As can be seen, the final calibration results for C, using either a 1- or 8-cross-validation, were very good. The better results using the 8-out cross-validation were unexpected and not readily explained. Even leaving out 16 samples resulted in satisfactory calibrations. Results for nitrogen were poorer than for C in all calibrations, but followed the same pattern. Finally, the addition of wavelengths from 400 to 1098 nm was of no benefit and actually resulted in higher calibration errors, as did the use of unground samples. Efforts with various data pre-treatments such as multiplicative scatter correction, mean centring etc., were not found to be of any benefit in efforts to improve calibrations using unground samples or wavelengths from 400 to 1098 nm. In Figure 1, the final calibration results for C for the 8-out cross-validation for the set of 64 ground samples are shown. As can be seen, despite the diversity of samples present, the results were excellent.

In Table 3, the calibration results achieved using various sample sets are shown. As indicated, the results for C were quite similar in the first study and for the initial set of 64 samples used here. The re-

Table 3. Final calibration results using various data sets and NIR spectra.

Source of calibration ^a	Carbon results			Nitrogen results		
	<i>R</i> ²	<i>RMSD</i> ^b	<i>RMSD</i> mean	<i>R</i> ²	<i>RMSD</i>	<i>RMSD</i> mean
Previous study	0.964	0.089	6.6	0.962	0.0074	6.2
Initial set of 64	0.926	0.118	7.4	0.892	0.0115	8.2
Initial set of 64	0.947	0.101	6.3	0.922	0.0098	7.0
Set of 547	0.824	0.232	19.4	0.783	0.0211	21.1
Set of 523	0.913	0.154	13.2	0.889	0.0144	14.7
Set of 509	0.918	0.146	12.6	0.903	0.0132	13.5

^aSee Table 1 for sample set identification, all results are for one-out cross-validations except for the second results for the set of 64 where an 8-out cross-validation was used (See Table 2).

^bRoot mean squared deviation.

results for N were not nearly as good as those for the set of 179 samples where the results for C and N were nearly identical (possibly due, at least in part, to the greater correlation between the two measures for the set of 179 samples, see Table 1). As indicated in the methods, after the success with the 64 samples, a more extensive set of 547 samples were collected from the same field. As shown in Table 3, the calibrations based on all 547 samples were not as good for either C or N. As seen in Figure 2 for C, many samples were indicated to be outliers, some concentration and some spectral or both. Removal of 24 and finally 38 samples (indicated to be concentration and/or

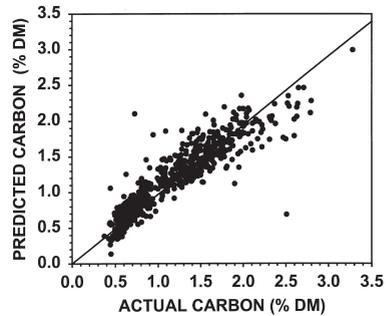


Figure 2. Final calibration results for C resulting from 1-out cross-validation analysis using set of 547 soil samples.

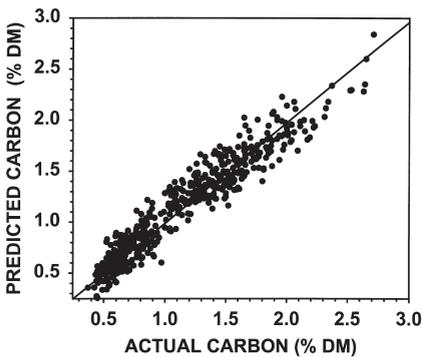


Figure 3. Final calibration results for C resulting from 1-out cross-validation analysis using set of 509 soil samples.

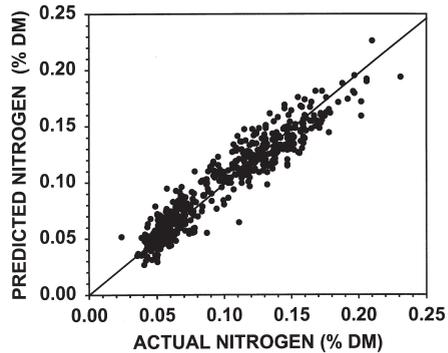


Figure 4. Final calibration results for N resulting from 1-out cross-validation analysis using set of 509 soil samples.

spectral outliers) resulted in sets of 523 and 509 samples, the results of which are also shown in Table 3. As shown, removal of samples resulted in considerable calibration improvement, but results were still not as good as for the set of 179 samples from Study 1 or the best results achieved with the initial set of 64 samples from the same fields (even compared with the results from the one-out cross-validation). This can also be seen in Figures 3 and 4 where the calibration results for C and N, using the set of 509 samples, are shown. The removal of so many samples as concentration outliers indicated that there may have been some quality control problems in the conventional determinations for C and N and this is being investigated. It is also possible that the less consistent grind produced by mortar and pestle is at least partially responsible and this also is being studied. However, these results still show that useful calibrations for C and N (especially C) are possible for soils of wide diversity.

Conclusions

Results of PLS calibrations have demonstrated that accurate calibrations for C, and to a lesser extent N, can be developed using NIR spectra for diverse sets of soil samples. However, these preliminary results indicate that calibrations developed using less diverse sets of soil samples may be more accurate. Results have also shown that, at least when scanned using a rotating sample cup, NIR calibrations worked considerably better when applied to ground soil samples. In conclusion, while further work is needed, results demonstrated that NIR can be extremely useful in the analysis of the large sample sets of soils required for spatial mapping studies.

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