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Predicting Decomposition Rates of Organic Resources Using Near Infrared Spectroscopy

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Abstract

Organic resources constitute a major source of nutrient inputs to both soils and livestock in smallholder tropical production systems. Information on decomposition characteristics is needed for sound management of organic resources. Measurement of C and N mineralisation rates and dry matter digestibility using current laboratory methods is both time-consuming and costly. This study tested near infrared (wavelengths from 1.0 to 2.5 μm) reflectance spectroscopy (NIRS) for rapid prediction of C and N mineralisation rates and in vitro dry matter digestibility for a diverse range of organic resources (n = 32). The organic resource samples were aerobically incubated in a sandy soil and amounts of C and N mineralised determined after 28 days. Organic resource attributes were calibrated to first derivative reflectance using partial least squares regression. Cross-validated r^2 values for actual versus predicted values were 0.82 for percentage of added C mineralised, 0.84 for percentage of added N mineralised, and 0.88 for in vitro dry matter digestibility. NIRS can be used for routine prediction of decomposition and nutrient release characteristics of organic resources. Construction of spectral calibration libraries in central laboratory facilities would greatly increase the efficiency of NIRS use for routine organic resource characterisation in laboratories throughout the world.

Organic resources constitute a major source of nutrient inputs to both soils and livestock in smallholder tropical production systems. The quality of organic resources regulates the potential rate of decomposition and availability of those nutrients, both in the soil and the rumen. Although the actual rate and degree of decomposition are moderated by the local activity of the decomposer organisms and the environmental conditions, plant litter quality is the factor most amenable to management in agricultural systems (Giller and Cadisch 1997; Heal et al. 1997). Recently, efforts have been undertaken to compile global information on decomposition and resource quality attributes as a basis for more systematic experimentation and development of predictive models (Palm et al. 2001). Using this diverse collection, Shepherd et al. (2004) demonstrated that near infrared spectroscopy (NIRS) can be used as a non-destructive method for rapid analysis of N, total soluble polyphenol and lignin concentration in organic resources. These quality attributes of organic resources largely determine their decomposition and nutrient release rates. The objectives of this study were to test the robustness of NIRS for direct prediction of C and N mineralisation rates and in vitro dry matter digestibility for a diverse set of samples from the organic resource database.

Methods

Thirty-two samples were selected from the organic resource database to represent a range of N, total soluble polyphenol and lignin concentrations (Gachengo et al. 2004b). The plant materials were aerobically incubated in sandy soil for 28 days as

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described by Gachengo et al. (2004a). The total amounts of C and N mineralised after 28 days were expressed as a percentage of their respective initial amounts added. The incubations were conducted in triplicate. In vitro dry matter digestibility was determined on the same materials in duplicate using standard methods (Barrios 2004). Diffuse reflectance spectra were recorded for each sample using a FieldSpecTM FR spectroradiometer (Analytical Spectral Devices Inc., Boulder, Colorado) at wavelengths from 1.0 to 2.5 µm, with a spectral sampling interval of 0.001 µm. Dried and ground (<1 mm) plant material was placed into 7.4 cm diameter Duran glass Petri dishes to a thickness of about 1 cm. The samples were scanned through the bottom of the Petri dishes using a high intensity source probe (Analytical Spectral Devices Inc., Boulder, Colorado). The probe illuminates the sample (4.5 W halogen lamp giving a correlated colour temperature of 3000 K; WelchAllyn, Skaneatles Falls, NY) and collects the reflected light from a 3.5 cm diameter sapphire window through a fibre-optic cable.

To sample within-dish variation, reflectance spectra were recorded at two positions, successively rotating the sample dish through 90º between readings. The average of 25 spectra (the manufacturer's default value) was recorded at each position to minimise instrument noise. Before reading each sample, 10 white reference spectra were recorded using calibrated spectralon (Labsphere®, Sutton, NH) placed in a glass Petri dish. Reflectance readings for each wavelength band were expressed relative to the average of the white reference readings. With this method, a single operator can comfortably scan 500 samples a day.

The raw spectral reflectance data were pre-processed before statistical analysis as follows. Relative reflectance spectra were resampled by selecting every hundredth-micrometre value from 1.0 to 2.5 µm. This was done to reduce the volume of data for analysis and to match it more closely to the spectral resolution of the instrument (0.003–0.01 µm). The reflectance values were then transformed with first derivative processing (differentiation with second-order polynomial smoothing with a window width of 0.02 µm) using a Savitzky-Golay filter, as described by Fearn (2000). Derivative transformation is known to minimise variation among samples caused by variation in grinding and optical set-up (Marten and Naes 1989). Multiplicative scatter correction (used to compensate for additive and/or multiplicative effects in spectral data) and normalisation (sample-wise scaling) of the reflectance data (both described in Vandeginste et al. (1998)) did not improve calibrations and so were not used. Wavebands in regions of low signal-to-noise ratio or displaying noise due to splicing between the individual spectrometers (Analytical Spectral Devices Inc. 1997) were omitted leaving 148 wavebands for analysis. The omitted bands were 1.00–1.01 µm, and 2.50 µm.

The data from the laboratory reference methods were calibrated against the reflectance wavebands using partial least squares regression, using 'The Unscrambler' (Camo ASA, Oslo) software. Hold-out-one full-cross validation was used to evaluate the stability of the calibrations. Jack-knifing was performed to eliminate unreliable (non-significant) wavebands, in order to simplify the final model and make it more reliable. Prediction success was evaluated on reference and actual observations using the coefficient of determination (r^2), root mean square error (RMSE) and bias.

Results and Discussion

Robust partial least squares calibrations were obtained for all the three reference methods (Table 1). There was more scatter in the calibration at low than high nitrogen mineralisation values (Figure 1), most likely reflecting imprecision in the laboratory

Table 1. Statistics for calibration and full-cross validation models for predicting decomposition reference values from near infrared reflectance.

Reference method	Calibration			Validation		
	r^2	RMSE	Bias	r^2	RMSE	Bias
C mineralisation	0.92	3.2	–8.9E-7	0.84	4.6	0.08
N mineralisation	0.89	13	1.7E-6	0.84	16	0.22
IVDM digestibility	0.95	3.9	–9.3E-7	0.88	6.3	–0.15

RMSE = root mean square error of calibration.
IVDM = in vitro dry matter digestibility.

measurements at very low plant nitrogen concentrations. The lowest calibration point for in vitro dry matter digestibility (sawdust sample) was underestimated in the cross-validated predictions (Figure 2). Having more samples with low digestibility in the calibration data set would improve the calibration.

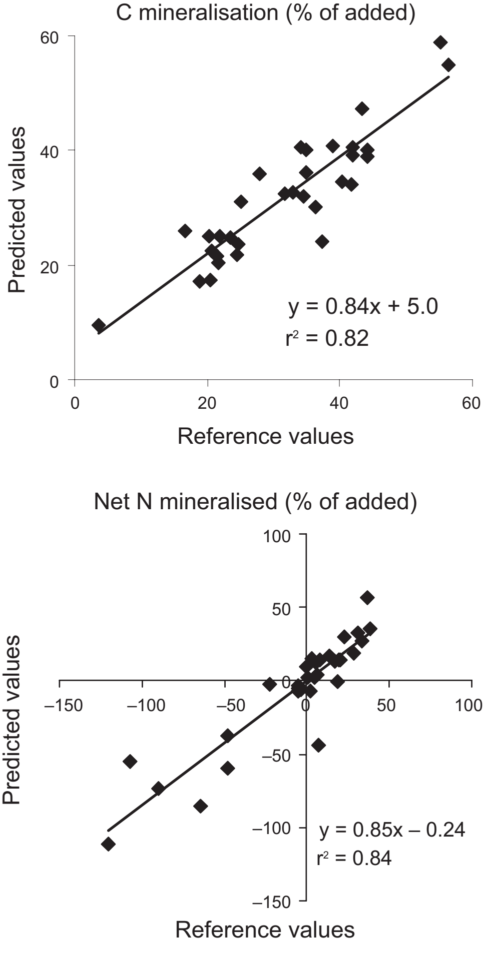

Figure 1. Spectrally predicted values versus laboratory reference values for amount of carbon and nitrogen mineralised from organic materials incubated in soil. The results are based on predictions using hold-out-one, full cross-validation.

Conclusion

NIRS shows promise for direct prediction of decomposition and nutrient-release characteristics of organic resources, obviating the need for tedious determination of organic resource attributes in the laboratory and the development of predictive models based on these attributes. Large spectral calibration libraries (Shepherd and Walsh 2002) for organic resources decomposition and nutrient-release characteristics should be built up in central laboratories. Then sets of standards will be all that is needed to cross-calibrate individual laboratory spectrometers to the central laboratory spectrometer. In this way, the efficiency of analysis of organic resource quality can be greatly increased. Further work should compare the accuracy and precision of the NIRS predictions of decomposition rates with predictions derived from attributes of organic resource quality determined by conventional laboratory methods, or with actual breakdown and related soil changes or growth responses in the field. The potential for widespread use of NIRS of measuring residue quality will increase as the laboratory uses for NIRS increase and the relative cost declines.

Acknowledgments

I thank Elvis Weullow for technical support on spectroscopy, Andrew Sila for assistance with data management, and gratefully acknowledge financial support from the Rockefeller Foundation.

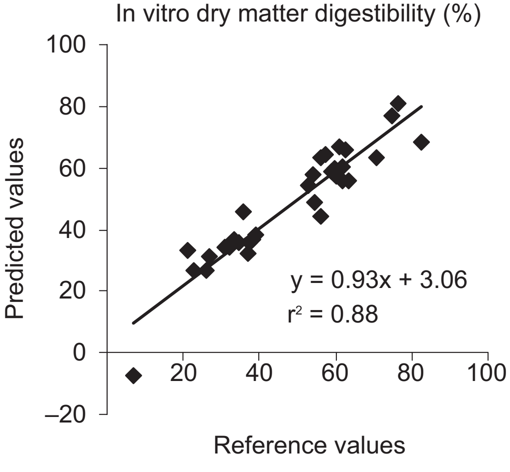

Figure 2. Spectrally predicted values versus laboratory reference values for in vitro dry matter digestibility of organic materials incubated in soil. The results are based on predictions using hold-out-one, full cross-validation

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