

Effect of soil texture on the prediction of soil parameters by near infrared spectroscopy

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Introduction

The movement of water and air through soil depends on soil porosity, which is controlled by the aggregation of soil components (e.g. carbon, nitrogen), clay minerals and organic matter (OM).¹ Sodium destroys soil structure by causing soil particles to repel each other and migrate into soil pores, hindering water and air transport.^{1,2} Excess soil sodium can arise from the use of high sodium irrigation water, and symptoms include pooling surface water and thinning turf. Calcium mitigates the negative effects of sodium and promotes soil aggregation by displacing sodium from soil particles, allowing it to be leached from the root zone with rainfall and irrigation.^{1,2}

Near infrared (NIR) spectroscopic data are often used to develop calibration models. There are a number of critical steps required to develop a calibration including sample selection, acquisition of spectra and reference data, pretreatment of spectral data, derivation of the regression model and validation of the model. However, the processing of the sample (e.g. grinding, drying), the intrinsic characteristics of the sample (e.g. sample matrix) and presentation of the sample to the instrument are important factors in the robustness and accuracy of NIR as analytical techniques.^{3,4} The aim of this study was to develop calibration models for sodium using NIR spectra, in order to evaluate the relationship between soil physical characteristics, Na and NIR.

Materials and Methods

Soil samples and reference analysis

Three hundred and thirty two (n = 332) soil samples were collected between 1997 and 1999 from different locations across Uruguay. Samples had different physical and chemical characteristics due to different soil types and management.⁵ Soil samples represent most of the agricultural soils in Uruguay (about 80%) and approximately 20% of the samples came from either sandy or red soils. Before soil analysis, samples were dried at 40°C in a forced-air oven for 24 h, and crushed and sieved through a 2 mm Wiley mill (Arthur H. Thomas, Swedesboro, NJ, USA).⁵ Physical and chemical characteristics of the soil samples analysed in this study were reported elsewhere.⁵ Sodium was analysed using methods reported elsewhere.²

Visible and NIR measurements

Dried soil samples were scanned for reflectance in a NIRSystems 6500 monochromator instrument (NIRSystems, Silver Spring, MD, USA). Soil samples (approx. 10 g) were placed into a small circular cuvette (55 mm diameter; NIRSystems IH-0307). The visible and NIR regions were collected (400–2500 nm) at 2 nm intervals using Infracore International software (ISI version 3.01, Infracore International, NIRSystems, Silver Spring, MD, USA), and the spectra were stored as the logarithm of the reciprocal of reflectance (Log 1/R).⁶ Samples were not rotated when spectra were collected.

Data analysis

Spectra were exported from the ISI software in NSAS format for chemometric analysis into The Unscrambler (version 7.5, CAMO ASA, Oslo, Norway). Calibration models between reference and NIR data were calculated using partial least squares (PLS) regression. The optimum number of terms (e.g. latent variables) in the PLS calibration models were determined by cross validation and defined by the PRESS (prediction residual error sum of squares) function in order to avoid overfitting. Due to the limited number of samples available with reference data, calibration models were developed and evaluated using full cross validation (leave one out method). Scatter correction used was achieved by applying the standard normal variate and detrend (SNV-D).⁷ The second derivative was used as a mathematical treatment to correct for

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baseline effects and to separate overlapping peaks, and was performed using Savitzky-Golay transformation (20 point and 2nd order filtering operation).

The NIR region (1100 to 2500 nm) was used to develop the calibration models. Statistics calculated included the coefficient of determination in calibration (R^2) and the root mean square of the standard error of cross validation (RMSECV). To evaluate the predictive ability of the PLS models, the residual predictive deviation (RPD), defined as the ratio between the standard deviation of the population (SD) and the RMSECV for the NIR calibrations, was also calculated.⁸ A NIR calibration is not considered robust if the error in estimation for a constituent (as measured by the RMSECV) is large compared with the spread in composition of that sample in the population (as SD): i.e. if the model has a relatively small RPD. An RPD greater than three is considered very good for prediction purposes.⁸

Results and Discussion

Table 1 shows the NIR cross validation statistics for Na concentration in the soil samples analysed, after mathematical transformation of the spectra using second derivative and SNV as scatter correction. The NIR calibration models developed for sandy soils explained more than 70% of variance in Y (Na concentration) accounted by X variables (NIR spectra), while only 40% of the variance was explained using the whole dataset. RPD values obtained were 1.1 and 1.8 for Na analysed in all and sandy soil samples, respectively. Regression coefficients for the PLS calibrations showed differences between the NIR calibrations obtained for Na concentration in soil and sandy soils, respectively. The highest regression coefficients for the calibration models developed using the whole dataset were around 1450 nm (OH second overtone, water), 1930 nm (OH first overtone, water), and around 2200 nm (aliphatic C-H and OH phenolic compounds). The highest coefficients for NIR calibrations of sandy soils were around 1950 nm (OH first overtone, water), 2070 nm and 2200 nm. These wavelengths are also associated with the absorption of crop and plant residues as well as with some oxides in the soil matrix.⁶

Table 1. Cross validation statistics for the measurement of Na concentration in arable soils using near infrared reflectance spectroscopy.

	R^2	RMSECV	LV	SD	RPD
All samples (n = 285)	0.42	0.12	5	0.14	1.1
Sandy soils (n = 47)	0.77	0.08	3	0.14	1.8

R^2 : coefficient of determination in calibration; RMSECV: root mean square of the standard error of prediction; LV; latent variables; SD: standard deviation; RPD: residual predictive deviation (SD/RMSECV).

Conclusion

This study suggested that soil texture (e.g. sand content) might influence the NIR calibration for the measurement of Na concentration in arable soils. The regression coefficients for each of the calibrations were different, indicating that some effect of the texture of the soils or other components of the soil matrix, affect the NIR calibrations for this parameter.

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