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Near Infrared Reflectance Spectroscopy (NIRS): prediction of chemical properties in Cuban soils

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Introduction

Soil chemical properties such as organic matter, phosphorus and potassium are important factors for soil fertility, successful plant growth and land management. Conventional methods to determine chemical fertility are often too difficult, costly, and time-consuming. Therefore economic and environmental conditions have promoted the development of new techniques of management agricultural systems. NIRS especially offers a wide range of in-line and at-line transmission and diffuse-reflection probes designed for the measurement of liquids and solids (Siesler, 2002) and is widely used in industry due to its simplicity, rapidness, and the need for little or no sample preparation (Chang et al., 2001). Hence allows significant advances in the area of food production with the application of agricultural inputs, such as fertilizers, seeds, pesticides, among other, in variable form inside a field, accordingly to the requirements or productive potential of several homogeneous sectors, pre-defined inside the same one. Thus, the modernization of agricultural practices arises as a new challenge, mainly in connection with the concept of environmental and economic sustainability of production process. NIRS in the context of precision agriculture might be an alternative to the conventional analyses methods employed in Cuba for determining these soil chemical properties by using a single spectrum per sample. The aim of this research was to build calibration and prediction models by correlating the chemical concentration of OM (%) and Olsen P; Oniani P; K₂O (mg 100g⁻¹ dry soil), determined by conventional methods in different soil samples, and the NIR reflectance spectra of these soil samples.

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Material and Methods

The whole process included sampling of Cambisols from different agricultural fields of Villa Clara province located at the central part of Cuba, chemical conventional analyses and soil reflectance measurements. Samples (189 split into 126 for calibration; 63 as test set) were air dried. The soil chemical properties content analyzed were organic matter (OM%- Walkley-Black); phosphorus (mg P 100g⁻¹ dry soil- Olsen and Oniani methods); potassium (mg K₂O 100g⁻¹ dry soil- Oniani method). These results are shown in Table 1.

The soil samples were scanning by means of a diode array spectrophotometer covering the wavelength range from 399 to 1697 nm. The pre-processing used were Log10 (1/R), Smoothing and Mean Center. The cross-validation strategy applied was Venetian blind. Calibration models were built using Partial Least Squares Regression (PLSR) for OM and Support Vector Machine (SVM) for Olsen P, Oniani P and K₂O. The prediction performance of the calibration models was evaluated based on the calibration statistics R^2 (the square of the correlation coefficient), RMSEP (root mean square error of prediction) and Bias (systematic deviation).

 Table 1. Reference data of the all soil samples analyzed with traditional laboratory analyses and scanned using NIRS

Soil property	Mean	Min	Max	S.D. (±)
OM (%)	2.95	2.23	3.98	0.42
Olsen P (mg 100g ⁻¹ dry soil)	2.55	1.68	4.10	0.58
Oniani P (mg 100g ⁻¹ dry soil)	12	5.10	25.02	5.36
K_2O (mg 100g ⁻¹ dry soil)	19.48	9.06	35.36	7.11

Min: minimum observed value; Max: maximum observed value; S.D. (±) - Standard deviation

Results and Discussion

During the analyses several samples were identified as outliers, or strange values whose presence could alter the results in a remarkable way, therefore were removed from the dataset. After the process of crossed validation Venetian blinds, significant coefficients (R^2) were obtained in all the soil properties analyzed in this research (Table 2).

The best prediction results based on the R^2 corresponded to the organic matter (R^2 = 0.91), followed by Olsen P and Oniani P both with R^2 = 0.80 and potassium (R^2 = 0.76). The lower values of RMSEC, RMSECV and RMSEP corresponded to the organic matter too.

Statistics	ОМ	Olsen P	Oniani P	K ₂ O
R^2 Cal	0.94	0.82	0.79	0.81
$R^2 CV$	0.93	0.79	0.75	0.75
\mathbf{R}^2 Pred	0.91	0.80	0.76	0.80
RMSEC	0.09	0.23	2.35	2.80
RMSECV	0.10	0.25	2.55	3.20
RMSEP	0.11	0.29	2.72	2.94
C Bias	0	5.5x10 ⁻⁴	0.16	-0.25
CV Bias	-0.00	1.8×10^{-3}	0.25	-0.09
Pred Bias	0.01	6.9×10^{-2}	0.27	0.10

Table 2. Statistics for NIRS predictions with PLSR and SVM analyses

 R^2 - square of the correlation coefficient of calibration (cal); cross validation (CV) and prediction (P); RMSE- root mean square error of calibration (cal); cross validation (CV) and prediction (Pred); Bias- systematic deviation

These results were in line with those obtained by Shao and He (2011). These authors reported R^2 equal to 0.82 and 0.80 for phosphorus and potassium respectively. Also, were in agreement with the results reported by He et al. (2005) for organic matter (R^2 = 0.96). On the other hand, were not in coincidence with the reported by Lee et al. (2003), due to they didn't obtain significant values for organic matter (R^2 = 0.49). The coefficients significance previously discussed were also demonstrated in figures 1 to 4. These figures show the relationship between the reference values obtained by means of conventional chemical analyses and the NIRS prediction.





Conclusions and Outlook

The soil chemical properties studied could be estimated with good and acceptable accuracy using either PLS or SVM regression analyses. The best prediction results were obtained for organic matter ($R^2>0.90$; RMSEP ≤ 0.11). The calibration and prediction models obtained might be an alternative for determining OM (%); Olsen P; Oniani P and K₂O (mg 100g⁻¹ dry soil) in Cuban agricultural soils. Finally, NIRS has the potential to rapidly determine the fertility of Cuban soils as an input to optimise the fertilisation in the future.

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