A. L. S. Santos[1], A. T. A. Linhares[2], P. H. C. G. Barbosa[3], W. R. C. Lopes[4], M. J. S. Reis[5], K. A. S. Rocha[6], D. G. de Oliveira[7], M. S. Rodrigues[8], D. S. Costa[9]

[1] Andreana Lima dos Santos e Santos: UNIVASF, Av. Antônio C. Magalhães, 510 - Santo Antônio, Juazeiro - BA, Brazil, 48902-300, e-mail: andreana.lima@discente.univasf.edu.br
[2] Adryelle Thayne Araújo Linhares: UNIVASF, Av. Antônio C. Magalhães, 510 - Santo Antônio, Juazeiro - BA, Brazil, 48902-300, e-mail: hemmolol1996@gmail.com
[3] Paulo Henrique Cunha Gonçalves Barbosa: UNIVASF, Av. Antônio C. Magalhães, 510 - Santo Antônio, Juazeiro - BA, Brazil, 48902-300, e-mail: paulo.gbarbosa@discente.univasf.edu.br
[4] Witor Reylan Carvalho Lopes: UNIVASF, Av. Antônio C. Magalhães, 510 - Santo Antônio, Juazeiro - BA, Brazil, 48902-300, e-mail: witor.reylan@discente.univasf.edu.br
[5] Maria José da Silva Reis: UNIVASF, Av. Antônio C. Magalhães, 510 - Santo Antônio, Juazeiro - BA, Brazil, 48902-300, e-mail: mariajose.reis@discente.univasf.edu.br
[6] Kátia Araújo da Silva Rocha: UNIVASF, Av. Antônio C. Magalhães, 510 - Santo Antônio, Juazeiro - BA, Brazil, 48902-300, e-mail: katia_a.s@outlook.com
[7] Deranor Gomes de Oliveira: UNIVASF, Av. Antônio C. Magalhães, 510 - Santo Antônio, Juazeiro - BA, Brazil, 48902-300, e-mail: deranor.oliveira@univasf.edu.br
[8] Marcos Sales Rodrigues: UNIVASF, Av. Antônio C. Magalhães, 510 - Santo Antônio, Juazeiro - BA, Brazil, 48902-300, e-mail: marcos.rodrigues@univasf.edu.br
[9] Daniel dos Santos Costa: UNIVASF, Av. Antônio C. Magalhães, 510 - Santo Antônio, Juazeiro - BA, Brazil 48902-300, e-mail: daniel.costa@univasf.edu.br

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DEVELOPMENT OF PREDICTIVE MODELS FOR DETERMINING ORGANIC CARBON AND CLAY CONTENT IN SOILS UNDER IRRIGATED FRUIT PRODUCTION IN THE BRAZILIAN SEMI-ARID REGION

Abstract.

The agricultural sector plays a central role in both greenhouse gas emissions and climate change mitigation through soil carbon sequestration. Total organic carbon (TOC) and soil texture, particularly clay content, are key indicators of this dynamic, as they influence organic matter stabilization, water retention, and soil structural quality. In semi-arid regions, where soil conditions, climate, and water scarcity impose limitations on agricultural production, the integrated assessment of these attributes is essential for sustainable management and low-carbon agriculture strategies. However, conventional laboratory methods for determining TOC and particle size distribution are costly, time-consuming, and dependent on the use of chemical reagents, which restricts their application in large-scale monitoring programs, especially for smallholder farmers. In this context, visible and near-infrared spectroscopy (Vis-NIR) stands out as a rapid and environmentally more sustainable alternative, enabling the simultaneous prediction of multiple soil attributes. Thus, the objective of this study was to develop statistical learning predictive models for the prediction of total organic carbon and clay contents in soils under irrigated fruit production systems in the Brazilian semi-arid region. The study was conducted in the Maniçoba Irrigation District, located in the municipality of Juazeiro, Bahia State, Brazil (9°20'05.13"S; 40°14'42.42"W). A total of 40 disturbed soil samples were collected at a depth of 0-0.3 m and analyzed using reference laboratory methods to determine total organic carbon and clay contents. Reflectance spectra were acquired within the 350-2500 nm range and subjected to different pre-processing strategies. Predictive modeling compared Principal Component Regression (PCR) and Partial Least Squares Regression (PLSR) models. Model performance was evaluated based on the coefficient of determination (R^2) and the root mean square error (RMSE) obtained through cross-validation. The results demonstrated that the PLSR model with orthogonal signal correction (OSC) pre-processing achieved the best performance for TOC ($R^2 = 0.887$; RMSE = 1.540) and clay ($R^2 = 0.960$; RMSE = 0.753) under reflectance mode. The application of OSC contributed to the removal of spectral variations not correlated with the response variable, thereby improving prediction accuracy. Therefore, Vis-NIR spectroscopy integrated with pre-processing and modeling strategies constitutes an efficient tool for the simultaneous prediction of TOC and clay, providing technical support for monitoring, reporting, and verification programs in low-carbon agriculture.

Keywords.
Irrigated agriculture; Vis-NIR spectroscopy; low-carbon fruit production; chemometrics.

Introduction

Global greenhouse gas (GHG) emissions reached approximately 59 billion tons of carbon dioxide equivalent (CO_2) in 2019, representing a 12% increase compared to 2010 (IPCC 2023). In this context, the agriculture, forestry, and other land use sector accounts for approximately 22% of global emissions, positioning agriculture as a strategic sector both in terms of emissions and its potential for climate change mitigation. In Brazil, this trend is even more pronounced. Data from the Greenhouse Gas Emissions and Removals Estimation System (SEEG 2023) indicate that emissions from agriculture and land-use change increased by 69% between 2010 and 2019, reinforcing the urgency of implementing low-carbon production systems.

The impacts of these emissions are particularly severe in the Brazilian semi-arid region. Between 1990 and 2020, the formation of arid areas was recorded in northern Bahia State (CEMADEN 2023), a region that hosts the São Francisco Valley fruit production hub. Despite its climatic vulnerability, the region has established itself as one of the country's leading agricultural production centers, particularly for crops cultivated under irrigated systems, whose cultivated areas comprise tens of thousands of hectares (IBGE 2022). However, maintaining competitiveness and access to international markets increasingly depends on demonstrating environmental sustainability and reducing the carbon footprint of agricultural production.

The integrated assessment of total organic carbon (TOC) content and soil texture, particularly the clay fraction, constitutes an important indicator of the quality and sustainability of agricultural systems, since the clay fraction plays a central role in the stabilization of soil organic matter through the formation of mineral-associated organic carbon, increasing its persistence and resistance to microbial decomposition, while also contributing to water retention and improved soil structure (MAO et al., 2024). However, the monitoring of these attributes remains limited by the high cost, analysis time, and dependence on laboratory infrastructure associated with conventional methods for determining organic carbon and particle-size distribution, which hinders the generation of datasets with high sampling density and the adequate representation of the spatial variability of agricultural soils (GRUSZCZYŃSKI; GRUSZCZYŃSKI, 2022). In this context, visible and near-infrared reflectance spectroscopy (Vis-NIR), combined with chemometrics, may represent an alternative for estimating soil properties in a rapid, non-destructive, and cost-effective manner (MUNNAF et al., 2022; SHIN et al., 2025). Therefore, the objective of this study was to develop statistical learning predictive models for predicting total organic carbon and clay contents in soils under irrigated fruit production systems in the Brazilian semi-arid region.

Materials and Methods

Study Area Description and Soil Sampling

The study was conducted in a rural community located within the Maniçoba Irrigation District, in the municipality of Juazeiro, Bahia State, Brazil (9°20'05.13"S; 40°14'42.42"W). The climate of the region is classified as hot semi-arid (BSh) according to the Köppen-Geiger classification system (ALVARES et al., 2013), with a mean annual temperature of 27 °C, mean annual relative humidity of 50%, mean annual precipitation of 500 mm, and mean annual evaporation of 2000 mm, indicating a high climatic water deficit (INMET, 2022; MOURA et al., 2023). The study area comprises different agricultural crops, with mango (Mangifera indica) production standing out for both domestic and international markets.

The experimental area comprises approximately 40 hectares. A sampling density of 1 sample per hectare was established, arranged in a regular grid. At each sampling point, soil samples were collected from the 0-0.3 m depth layer. Furthermore, a stratified sampling approach (canopy projection vs. inter-row area) was adopted considering the high spatial variability of soil attributes in perennial fruit production systems (ARAÚJO, 2021).

Laboratory Analyses

Disturbed soil samples were collected from the 0-0.3 m soil layer. The samples were air-dried, gently crushed, and passed through a 2.0 mm sieve to obtain Air-Dried Fine Earth (ADFE). Using the ADFE fraction, soil particle-size distribution was determined by the pipette method (TEIXEIRA et al., 2017). Total Organic Carbon (TOC) was determined using the wet digestion method with an acidified potassium dichromate solution, followed by heating and titration of the excess potassium dichromate with an ammonium ferrous sulfate solution, according to Yeomans and Bremner (1988).

Vis-NIR Spectra Acquisition

For spectral data acquisition, 10 cm^3 of Air-Dried Fine Earth (ADFE) samples were used (VISCARRA ROSSEL et al., 2016). The Vis-NIR reflectance spectra of the samples were acquired using a FieldSpec 3 spectroradiometer (Analytical Spectral Devices, Boulder, Colorado, USA), equipped with an optical sensor operating in the spectral range from 350 to 2500 nm, with a spectral resolution of 8 nm and an accuracy of ± 1 nm. The instrument was coupled to a Muglight probe equipped with a 4 W quartz-tungsten-halogen lamp and connected to a computer running RS3 software (Analytical Spectral Devices, Boulder, Colorado, USA). In addition, a white reference panel was used, with optimization and calibration procedures performed prior to spectral data acquisition. Each spectrum for each soil sample consisted of the average of 30 scans performed by the instrument. Reflectance values were obtained and used to construct the mean spectral curves of the soil samples. Subsequently, the reflectance values were transformed into absorbance measurements (log(1/R)), where R represents reflectance, using ViewSpec Pro software (Analytical Spectral Devices, Boulder, Colorado, USA). Both reflectance and absorbance data were used for the development of the chemometric models.

Development of Predictive Models

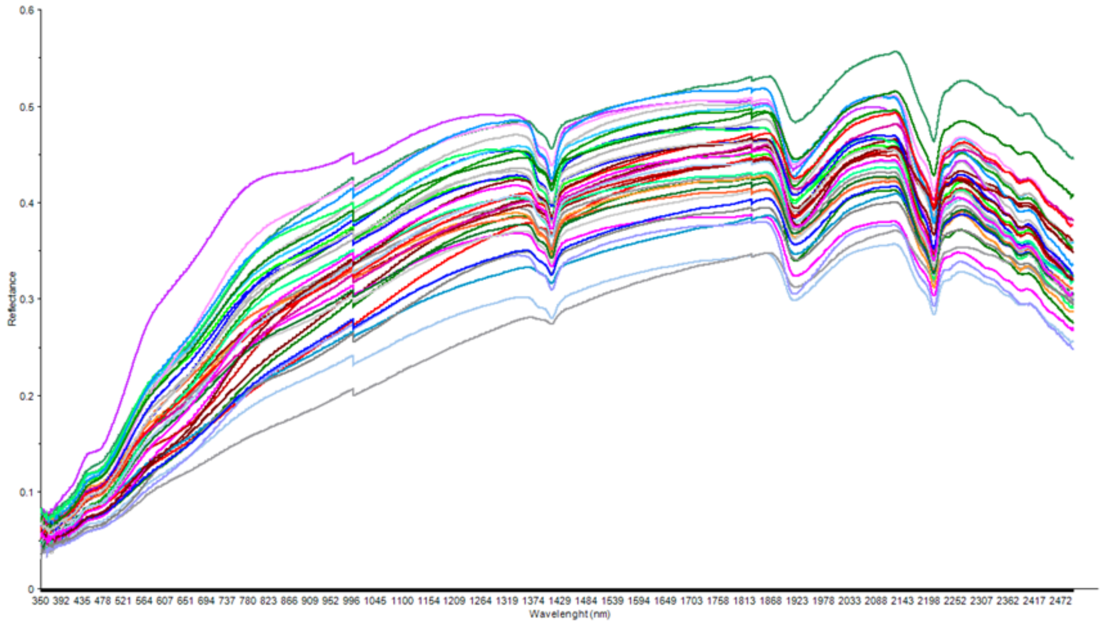
The acquired spectra underwent several pre-processing procedures. Raw data were subjected to normalization, first- and second-order Savitzky-Golay derivatives (GORRY, 1990) using second-order polynomials, Multiplicative Scatter Correction (MSC) (ISAKSSON; NAES, 1988), Standard Normal Variate (SNV) transformation (BARNES et al., 1989), and Orthogonal Signal Correction (OSC) (WOLD et al., 1998).

For modeling purposes, the matrices containing the spectral data were used as independent predictor variables (X matrix), while total organic carbon (TOC) content and clay content were used as dependent response variables (Y vector). The chemometric models were developed using all samples available in the dataset. Predictive performance was evaluated through full cross-validation (MARTENS; DARDENNE, 1998).

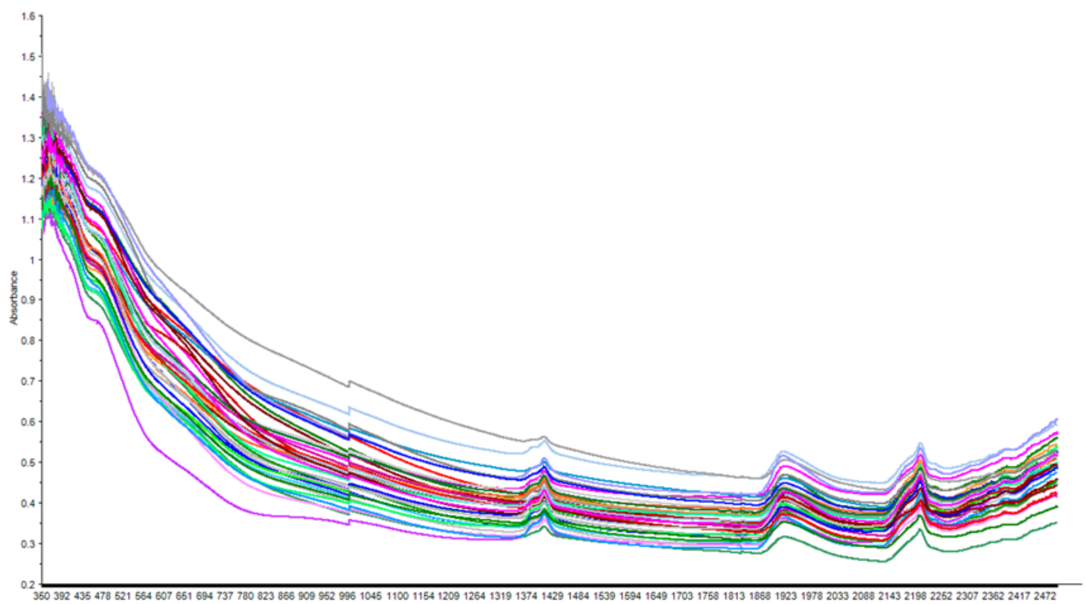
The construction of predictive models relating spectral data to total organic carbon and clay contents involved different algorithms, including Principal Component Regression (PCR) and Partial Least Squares Regression (PLSR). Model accuracy was assessed using the following statistical metrics: calibration coefficient of determination (R^2C); root mean square error of calibration (RMSEC); standard error of calibration (SEC); cross-validation coefficient of determination (R^2CV); root mean square error of cross-validation (RMSECV); and standard error of cross-validation (SECV).

Results and Discussion

Figures 1a and 1b show the spectral behavior of the soil samples in reflectance and absorbance modes, respectively. The need for spectral signal pre-processing is evident, as indicated by the slope and displacement of the baseline, as well as spectral signal scattering. No evident spectral features were observed in the visible (Vis; 350–700 nm) and near-infrared (NIR; 701–1100 nm) regions. Thereafter, in the short-wave infrared region (SWIR; 1101–2500 nm), the spectrum was characterized by prominent spectral signatures located around 1400, 1950, and 2200 nm.



(a)



(b)

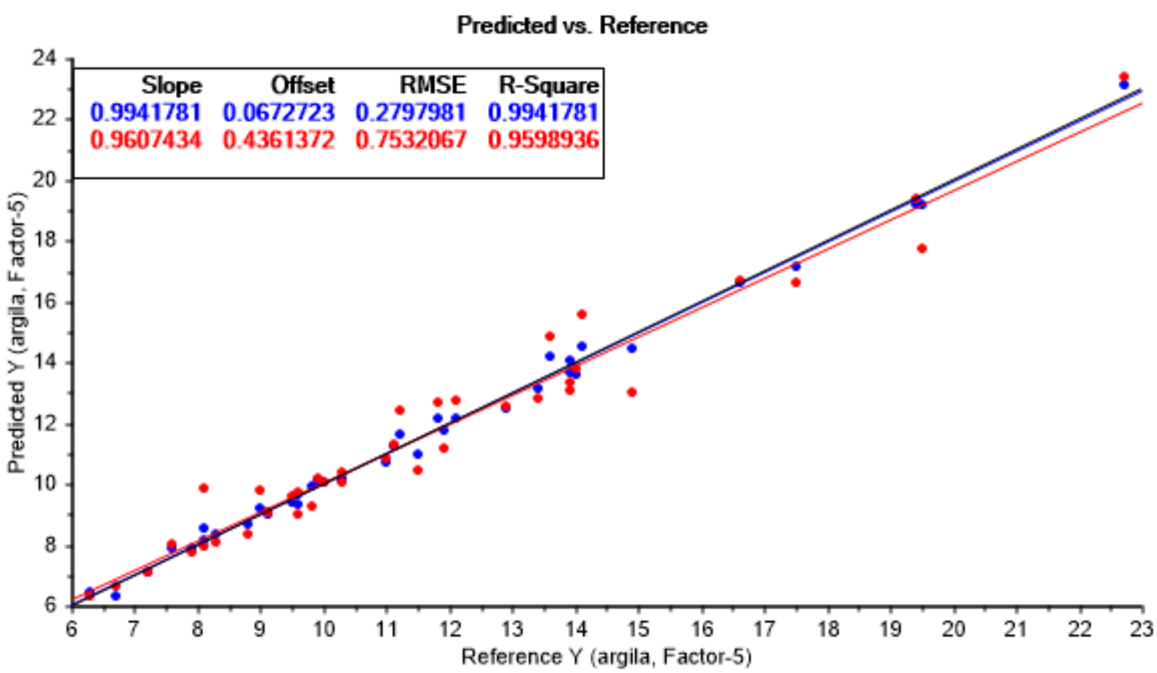
Fig 1. Spectra of (a) reflectance and (b) average absorbance of soil samples in the 0.00-0.30 depth layers in irrigated fruit-growing production areas in the Brazilian semi-arid region.

For clay content, the Partial Least Squares Regression (PLSR) model associated with Orthogonal Signal Correction (OSC) pre-processing was the model that exhibited the best performance in both reflectance and absorbance modes (Table 1). The PLSR model with OSC in reflectance mode achieved an R^2CV of 0.960, an RMSECV of 0.753, and an SECV of 0.763 (Figure 2a). The

PLSR model with OSC in absorbance mode achieved an R^2CV of 0.933, an RMSECV of 0.970, and an SECV of 0.982 (Figure 2b).

Table 1. Parameters of PCR and PLSR regression models associated with different pre-processing methods, in reflectance and absorbance modes, for clay content of soils used in irrigated fruit farming in the semi-arid region of Brazil.

Model Clay	R2cal	RMSEC	SEC	R2cv	RMSECV	SECV
PCR_ref_raw	0.810	1.597	1.617	0.764	1.828	1.851
PCR_ref_Normalize	0.731	1.900	1.924	0.649	2.226	2.254
PCR_ref_SGolay	0.821	1.552	1.572	0.761	1.838	1.859
PCR_ref_2SGolay	0.638	2.206	2.234	0.595	2.392	2.422
PCR_ref_SNV	0.785	1.702	1.724	0.726	1.969	1.994
PCR_ref_MSC	0.816	1.573	1.593	0.741	1.915	1.938
PCR_ref_OSC	0.928	0.986	0.998	0.915	1.096	1.109
PCR_abs_raw	0.776	1.734	1.756	0.669	2.165	2.191
PCR_abs_Normalize	0.784	1.705	1.727	0.715	2.007	2.033
PCR_abs_SGolay	0.698	2.016	2.042	0.654	2.213	2.241
PCR_abs_2SGolay	0.000	3.667	3.714	NA	3.821	3.869
PCR_abs_SNV	0.806	1.615	1.635	0.745	1.899	1.924
PCR_abs_MSC	0.793	1.669	1.691	0.728	1.961	1.986
PCR_abs_OSC	0.849	1.422	1.440	0.833	1.538	1.558
PLSR_ref_raw	0.824	1.539	1.559	0.762	1.835	1.858
PLSR_ref_Normalize	0.847	1.433	1.452	0.723	1.978	2.000
PLSR_ref_SGolay	0.882	1.257	1.273	0.815	1.616	1.636
PLSR_ref_2SGolay	0.669	2.111	2.138	0.593	2.399	2.429
PLSR_ref_SNV	0.828	1.520	1.539	0.747	1.893	1.917
PLSR_ref_MSC	0.847	1.436	1.454	0.747	1.890	1.913
PLSR_ref_OSC	0.994	0.280	0.283	0.960	0.753	0.763
PLSR_abs_raw	0.802	1.633	1.654	0.678	2.136	2.162
PLSR_abs_Normalize	0.815	1.578	1.598	0.719	1.992	2.017
PLSR_abs_SGolay	0.918	1.047	1.061	0.719	1.993	2.019
PLSR_abs_2SGolay	0.882	1.262	1.278	0.496	2.670	2.703
PLSR_abs_SNV	0.829	1.516	1.536	0.761	1.841	1.864
PLSR_abs_MSC	0.877	1.286	1.302	0.761	1.838	1.861
PLSR_abs_OSC	0.978	0.538	0.545	0.933	0.970	0.982



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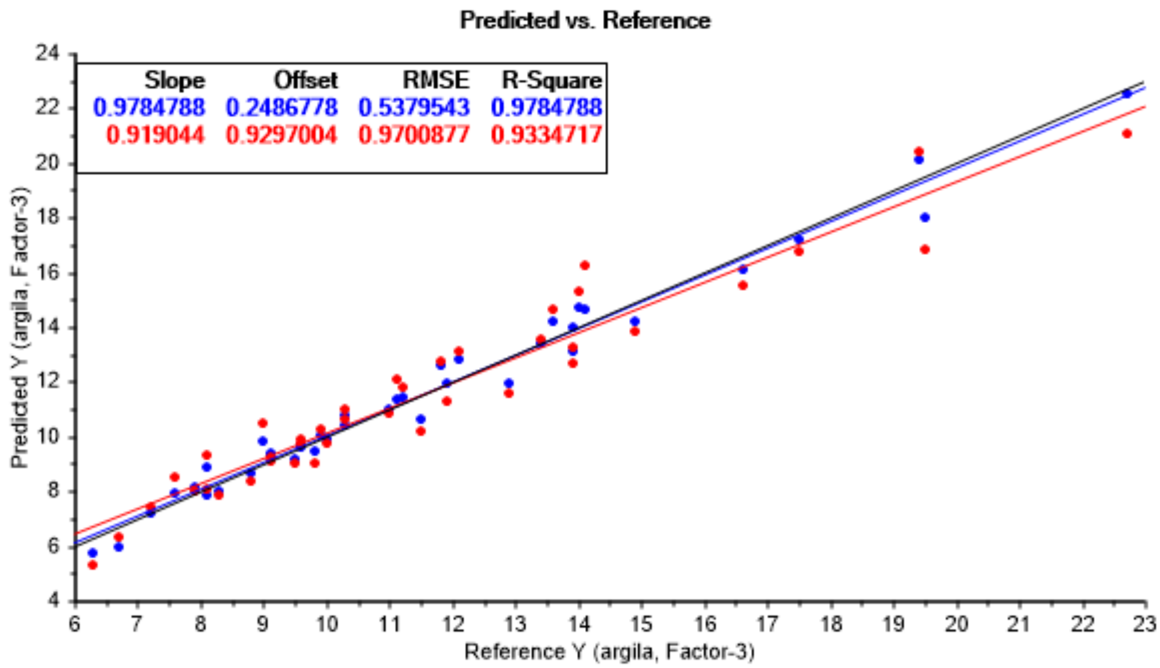


(b)

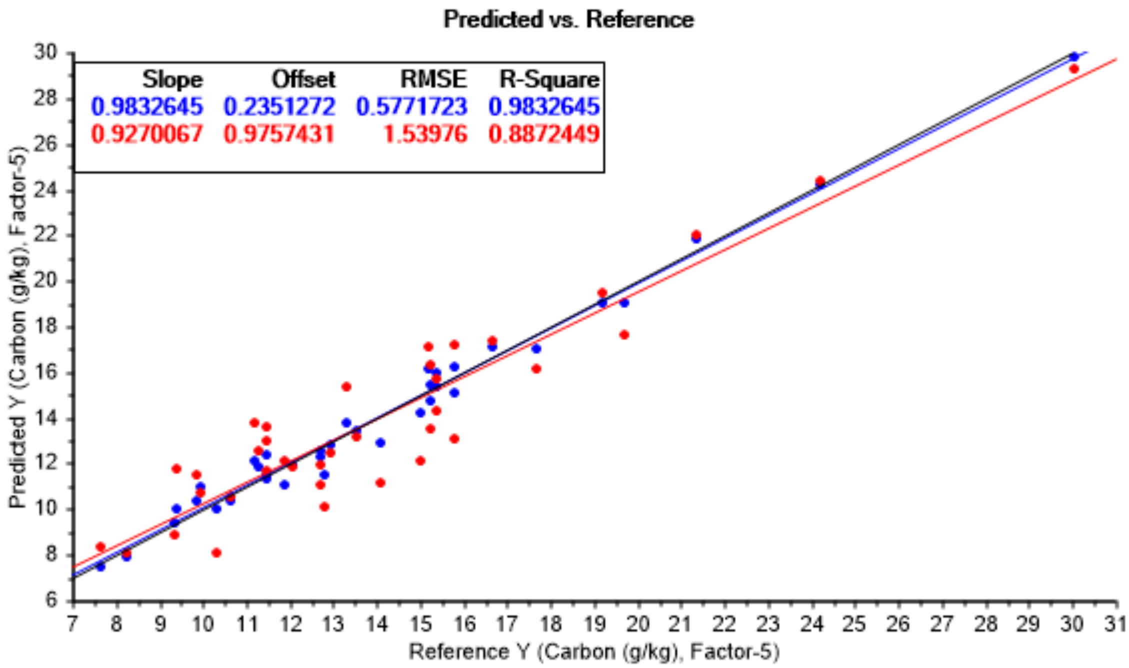
Fig 2. Scatter plot of PLSR models associated with OSC pre-processing in reflectance and absorbance mode for clay content.

For total organic carbon content, the Partial Least Squares Regression (PLSR) model associated with Orthogonal Signal Correction (OSC) pre-processing was the model that exhibited the best performance in both reflectance and absorbance modes (Table 2). The PLSR model with OSC in reflectance mode achieved an R^2CV of 0.887, an RMSECV of 1.540, and an SECV of 1.560 (Figure 3a). The PLSR model with OSC in absorbance mode achieved an R^2CV of 0.782, an RMSECV of 2.142, and an SECV of 2.172 (Figure 3b).

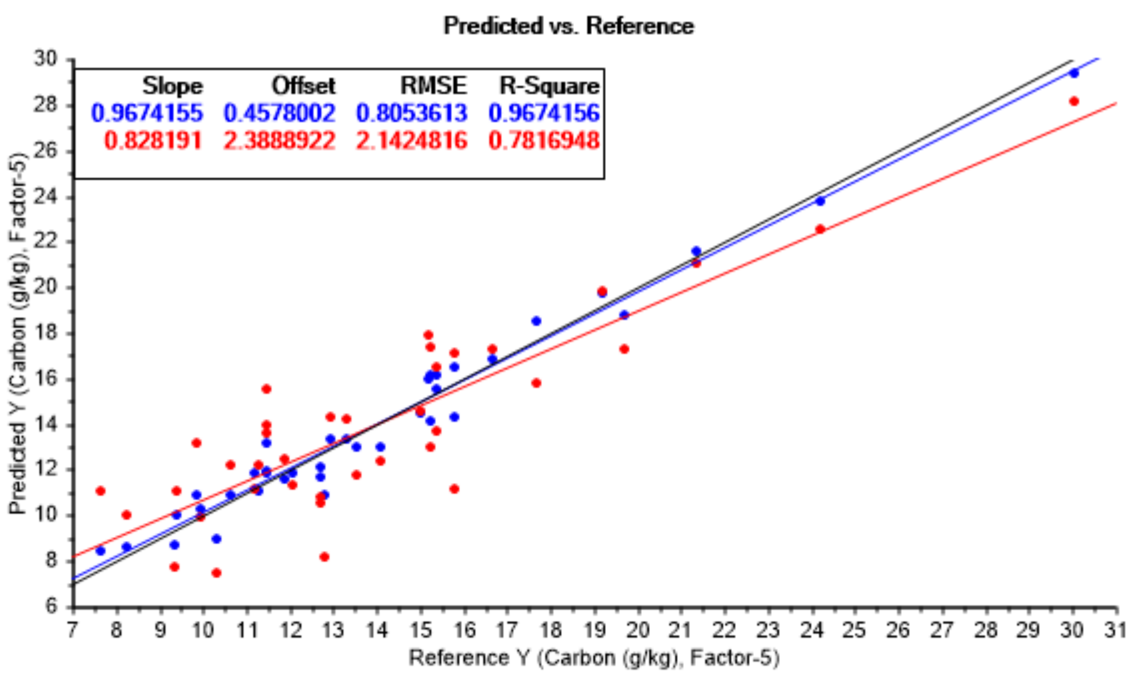
Table 2. Parameters of the PCR and PLSR regression models associated with different pre-processing methods, in reflectance and absorbance modes, for total organic carbon content of soils from irrigated fruit farming in the Brazilian semi-arid region.

Model Carbon	R2cal	RMSEC	SEC	R2cv	RMSECV	SECV
PCR_ref_raw	0.338	3.631	3.681	0.223	4.043	4.098
PCR_ref_Normalize	0.309	3.708	3.759	0.223	4.041	4.097
PCR_ref_SGolay	0.414	3.416	3.463	0.313	3.801	3.853
PCR_ref_2SGolay	0.398	3.460	3.508	0.317	3.790	3.842
PCR_ref_SNV	0.561	2.957	2.998	0.351	3.694	3.743
PCR_ref_MSC	0.528	3.065	3.107	0.326	3.765	3.815
PCR_ref_OSC	0.770	2.140	2.170	0.715	2.448	2.482
PCR_abs_raw	0.393	3.475	3.523	0.283	3.883	3.936
PCR_abs_Normalize	0.527	3.067	3.109	0.232	4.019	4.071
PCR_abs_SGolay	0.425	3.384	3.431	0.316	3.791	3.842
PCR_abs_2SGolay	0.301	3.730	3.782	0.114	4.315	4.373
PCR_abs_SNV	0.547	3.004	3.045	0.373	3.631	3.678
PCR_abs_MSC	0.545	3.008	3.050	0.377	3.619	3.666
PCR_abs_OSC	0.809	1.949	1.976	0.717	2.438	2.470
PLSR_ref_raw	0.599	2.827	2.866	0.292	3.858	3.911
PLSR_ref_Normalize	0.325	3.666	3.717	0.237	4.004	4.059
PLSR_ref_SGolay	0.483	3.208	3.252	0.313	3.800	3.853
PLSR_ref_2SGolay	0.421	3.395	3.441	0.297	3.845	3.898
PLSR_ref_SNV	0.586	2.871	2.911	0.249	3.973	4.026
PLSR_ref_MSC	0.575	2.908	2.948	0.340	3.726	3.777
PLSR_ref_OSC	0.983	0.577	0.585	0.887	1.540	1.560
PLSR_abs_raw	0.357	3.578	3.627	0.256	3.955	4.009
PLSR_abs_Normalize	0.220	3.941	3.996	0.129	4.278	4.337

PLSR_abs_SGolay	0.501	3.150	3.194	0.322	3.775	3.826
PLSR_abs_2SGolay	0.551	2.990	3.031	0.132	4.271	4.322
PLSR_abs_SNV	0.690	2.486	2.520	0.349	3.700	3.749
PLSR_abs_MSC	0.707	2.417	2.450	0.428	3.467	3.506
PLSR_abs_OSC	0.967	0.805	0.816	0.782	2.142	2.172



(a)



(b)

Fig 3. Scatter plot of PLSR models associated with OSC pre-processing in reflectance and absorbance mode for total organic carbon content.

The high coefficients of determination observed for clay prediction demonstrate the strong relationship between the soil spectral response and its textural composition. Similar results were reported by Silva et al. (2024), who verified the efficiency of VIS-NIR-SWIR spectroscopy in estimating clay content and in the textural classification of soils for agricultural applications. Complementarily, Silva-Sangoi et al. (2024) obtained coefficients of determination of up to 0.95 for clay prediction using Vis-NIR-SWIR spectroscopy associated with spectral pre-processing techniques. These results corroborate the findings of the present study and reinforce the potential of spectroscopy as a rapid, non-destructive, and lower-cost alternative for soil textural characterization, particularly in semi-arid regions and irrigated agricultural systems.

The application of Orthogonal Signal Correction (OSC) promoted significant improvements in the performance of the developed models, resulting in increases in the coefficients of determination and reductions in cross-validation errors for both evaluated attributes. This behavior is consistent with the results obtained by Biney et al. (2021), who compared OSC with nine traditional spectral pre-processing techniques and found a consistent superiority of the method for soil organic carbon prediction. According to the authors, OSC removes spectral components orthogonal to the response variable, reducing interferences related to light scattering, instrumental noise, and variations not associated with the attribute of interest. The improvement observed in this study suggests that part of the variability present in the original spectra was not directly related to clay and total organic carbon contents and was efficiently removed by OSC. Therefore, the results reinforce the importance of spectral pre-processing in the construction of robust chemometric models and demonstrate the potential of OSC for applications in soil spectroscopy.

Conclusion

Visible and near-infrared spectroscopy (Vis-NIR), when integrated with pre-processing strategies and multivariate modeling, proved to be a promising tool for the simultaneous determination of total organic carbon and clay contents in soils under irrigated agriculture in the Brazilian semi-arid region, offering technical support for monitoring, reporting, and verification programs in low-carbon agriculture.

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