

# Soil characterization by near-infrared spectroscopy and principal component analysis<sup>1</sup>

## Caracterização de solos por espectroscopia no infravermelho próximo e análise de componentes principais

Maria Ivanilda de Aguiar<sup>2\*</sup>, Lívia Paulia Dias Ribeiro<sup>3</sup>, Aurea Pinto dos Ramos<sup>2</sup> and Edson Lopes Cardoso<sup>2</sup>

**ABSTRACT** - This research aimed to use principal component analysis (PCA) as an exploratory method for spectral data of soil absorbance from the Baturité Massif and Central Hinterland (Ceará State, Brazil) to verify the potential of the technique in soil characterization. We analyzed 46 soil samples from different areas (native and cultivated). Each sample was analyzed in two particle sizes: 2 and 0.2 mm. We obtained spectral data by near-infrared spectroscopy (NIR), selecting the 1,360–2,260 nm range (2,376 variables). We evaluated three data pretreatment methods: multiplicative scatter correction (MSC), first derivative, and second derivative of the Savitzky-Golay filter. The absorption bands observed were: 1,414 nm (C–H stretching and deformation combination), 1,450 nm (O–H associated with the carbon chain), 1,780 nm (second overtone of C–H), 1,928 nm (O–H associated with molecular water), and 2,208 nm (C–H stretch and C=O combination). The best pretreatment was verified using only the multiplicative scatter correction (MSC). Two principal components explained 98% of the data variability, being the first principal component (PC1) related to the characteristic band of moisture, with negative values in the 1,928 nm region, while the second principal component (PC2) was related to the total organic matter (OM) originating from the C–H, C=O, and N–H bonds, wavelength region 1,414 nm. The PCA allowed characterizing the samples in terms of moisture and OM contents, with emphasis on soils under irrigated agroforestry system with higher values of moisture and OM, while the soil in degradation process presented lower values for these attributes. The NIR spectroscopy, associated with data processing methods (PCA and MSC), allows identifying changes in soil attributes, such as moisture and OM.

**Keywords:** Non-destructive analysis. Soil spectral response. Particle size.

**RESUMO** - Objetivou-se empregar Análise de Componentes Principais (PCA) como ferramenta exploratória dos dados espectrais de absorbância de solos do Maciço de Baturité e do Sertão Central (Ceará, Brasil), para verificar a potencialidade da técnica na caracterização dos solos. Foram analisadas 46 amostras oriundas de solos de diferentes áreas (cultivadas e nativas). Cada amostra foi analisada em duas granulometrias, 2 e 0,2 mm. Os dados espectrais foram obtidos pela espectroscopia no infravermelho próximo (NIR), selecionando-se a faixa 1.360 a 2.260 nm (2.376 variáveis). Avaliou-se três pré-tratamentos dos dados: correção do espalhamento de luz (MSC), 1ª e 2ª derivadas Savitzky-Golay. Foram observadas as bandas de absorção: 1.414 nm (C-H combinação de estiramento e deformação), 1.450 nm (O-H associado à cadeia carbônica), 1.780 nm (2º sobretono C-H), 1.928 nm (O-H associado à água molecular) e 2.208 nm (C-H estiramento e C=O combinação). O melhor pré-tratamento foi verificado usando apenas a correção de espalhamento de luz (MSC). Dois componentes principais explicaram 98% da variabilidade dos dados, sendo que a primeira componente principal (PC1) foi relacionada com a banda característica de umidade, com valores negativos na região de 1.928 nm, enquanto a segunda componente principal (PC2) foi relacionada à matéria orgânica total (MO) oriunda das ligações C-H, C=O e N-H, região do comprimento de onda 1.414 nm. A PCA permitiu caracterizar as amostras quanto a umidade e teores de MO, destacando-se os solos sob sistema agroflorestal irrigado com maiores valores de umidade e MO, enquanto o solo em processo de degradação apresentou menores valores para estes atributos. A espectroscopia NIR associada às ferramentas de tratamentos de dados (PCA e MSC) permite identificar alterações em atributos do solo, como umidade e MO.

**Palavras-chave:** Análise não destrutiva. Resposta espectral do solo. Tamanho de partícula.

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\* Author for correspondence.

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<sup>2</sup>Instituto de Desenvolvimento Rural, Universidade da Integração Internacional da Lusofonia Afro-Brasileira/UNILAB, Rua José Franco de Oliveira, s/n, Redenção-CE, Brasil, 62.790-970, ivanilda@unilab.edu.br (ORCID ID 0000-0002-6147-2621), aureapinto44@gmail.com (ORCID ID 0000-0003-4382-9671), edsoncardoso89@hotmail.com (ORCID ID 00 00-0001-5400-8938)

<sup>3</sup>Instituto de Ciências Exatas e da Natureza, Universidade da Integração Internacional da Lusofonia Afro-Brasileira/UNILAB, Redenção-CE, Brasil, liviapaulia@unilab.edu.br (ORCID ID 0000-0003-3067-1908)

## INTRODUCTION

The determination of soil properties is important to monitor its quality, aiming at the sustainability of the activities developed in it. Conventional soil analysis methods take time, require equipment that demands high initial investments, and, in general, use chemical reagents, generating waste that needs proper treatment and disposal (MIYAZAWA; VIEIRA; ARAUJO-JUNIOR, 2019; SORIANO-DISLA *et al.*, 2014).

In order to meet the demands of soil analysis, it is essential to develop new methodologies that are fast and have lower cost and lower environmental impact. In this sense, analyses by means of remote sensing techniques have gained prominence, more specifically using the visible and infrared regions close to the electromagnetic spectrum (ARAÚJO; DEMATTÊ; BELLINASSO, 2013; RECENA; FERNÁNDEZ-CABANÁS; DELGADO, 2019).

Near-infrared spectroscopy (NIR) has been used in the development of methods for quantifying organic compounds and identifying spectral patterns for sample characterization. NIR spectroscopy allows a greater depth of penetration into samples and subsequent possibilities for fast, non-destructive, and chemical-free analyses (MANLEY, 2014). Thus, its use in soil science has gained prominence in recent years because spectral profiles are correlated with the physical, chemical, and biological characteristics of the soil (DEMATTÊ *et al.*, 2015; FELIX *et al.*, 2016; MANLEY, 2014; RECENA; FERNÁNDEZ-CABANÁS; DELGADO, 2019; TERRA; DEMATTÊ; VISCARRA ROSSEL, 2015; ULUSOY *et al.*, 2016).

The use of NIR spectroscopy is conducive to monitoring soil quality in management systems. However, there is a need to implement soil spectral data libraries to facilitate the interpretation of spectral responses of the wide diversity of soils in Brazil (DEMATTÊ *et al.*, 2015). For this, studies are necessary to allow a broad characterization of soils, as there is a lack of information, especially in the Northeast of Brazil.

On the other hand, it is important to consider the way of preparing the sample for spectral data collection, as it is possible to observe protocol variations for direct spectroscopy of soil, without standardization regarding the size of the analyzed particles (BEN DOR; ONG; LAU, 2015). Some studies indicate the influence of soil particle size on spectral responses, with better results in reduced sizes (BARTHÈS *et al.*, 2008; FELIX *et al.*, 2016; SORIANO-DISLA *et al.*, 2014). Thus, we need further studies to identify the relationship between the particle size of the samples and soil spectral responses.

In soil direct spectroscopic analysis by diffuse reflectance, it is essential to use spectral data pretreatment

methods due to the divergent behavior of the spectra concerning the baseline, mainly explained by the scattering of light. In this case, data processing improves the accuracy of the models by removing unwanted side effects and by accentuating spectral characteristics (HONG *et al.*, 2019). As options of pretreatment, we can mention the multiplicative scatter correction (MSC) and first and second derivatives of the Savitzky-Golay filter (XU *et al.*, 2018).

After pretreatment, it is necessary to analyze the data, and principal component analysis (PCA) is one of the most used methods to visualize spectral patterns and structures of different samples, revealing their similarities and differences, evidencing the potential for soil characterization through its spectral data by segregating samples with different characteristics.

This study is based on the hypotheses that NIR absorption bands can detect differences in soil composition under different uses, allowing their characterization, and that the particle size of the soil can interfere in its spectral response. The objective was to use principal component analysis (PCA) as a method for characterization and identification of a spectral pattern of absorbance of soil samples collected in areas submitted to different managements, in order to verify the potential of the technique (PCA of spectral data) for soil characterization. The research also aimed to determine whether there is a relationship between the particle size and the spectral response of the soil.

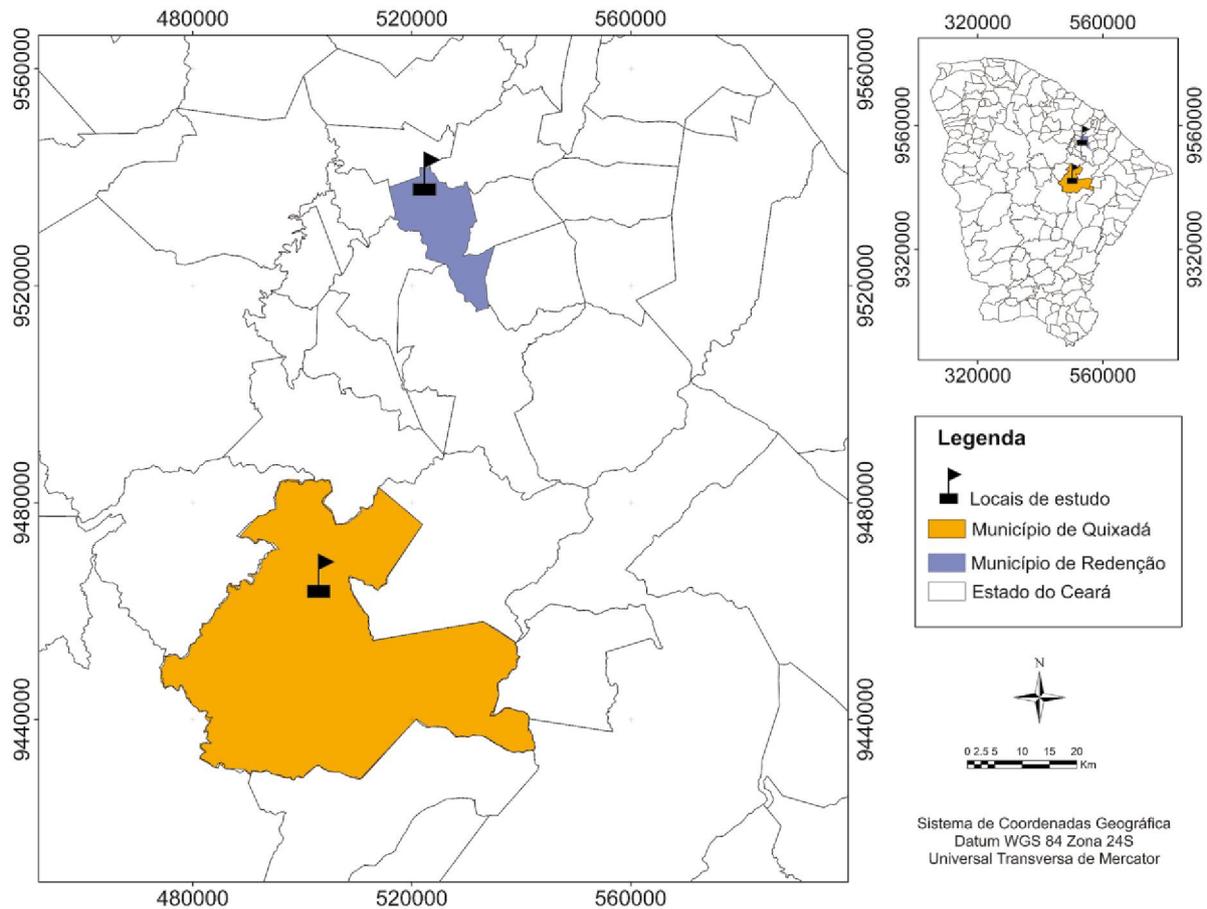
## MATERIAL AND METHODS

### Places of collection, sampling, and preparation of samples

We studied 46 soil samples from the cities of Redenção and Quixadá, located in the regions of the Baturité Massif and the Central Hinterland, Ceará State, Brazil (Figure 1). In Redenção, the collection was made at Fazenda Experimental Piroás (FEP/UNILAB) and in family farming areas near this location.

The climate in Redenção can be classified as Hot-Humid Tropical, Hot Sub-humid Tropical, or Mild Hot Semi-Arid Tropical. The average temperature ranges from 26 to 28 °C, and the average annual precipitation is 1,062 mm, with a rainy season from January to April. The predominant soils are Planosols and Luvisols (INSTITUTO DE PESQUISA E ESTRATÉGIA ECONÔMICA DO CEARÁ, 2017a; SANTOS *et al.*, 2018).

In Quixadá, the collection was carried out at Fazenda Não Me Deixes. The climate is classified

**Figure 1** - Collection sites of the evaluated soils

as Hot Semi-Arid Tropical, with an average annual rainfall of 838.1 mm, concentrated from February to April, and the average annual temperature ranges from 26 to 28 °C (INSTITUTO DE PESQUISA E ESTRATÉGIA ECONÔMICA DO CEARÁ, 2017b). Luvisols, Entisols, Planosols and Acrisols predominate in Quixadá (INSTITUTO DE PESQUISA E ESTRATÉGIA ECONÔMICA DO CEARÁ, 2017a; SANTOS *et al.*, 2018).

In Redenção, we collected 30 soil samples in areas under the following managements: rice and corn — traditional rice and corn cultivation in its first year after deforestation and burning of vegetation; pasture — pasture with more than five years of management, maintained without irrigation, grazed by sheep; Caatinga — area under native Caatinga vegetation in the secondary succession of approximately eight years; coffee\_AFS — coffee cultivation in an agroforestry system (coffee shaded by native Atlantic Forest species); rice\_AFS — rice cultivation (dryland

farming) in agroforestry system, second year of implantation; and irrigated rice\_AFS — cultivation of irrigated rice in agroforestry system, first year. We collected five samples (of approximately 1 kg) in each area, in the 0.0–0.1 m layer, from October to December 2018. In Quixadá, we collected 16 samples in the Caatinga area under degradation process, after traditional cultivation of the soil (cutting and burning) under dryland conditions. We collected samples in the 0.0–0.1 m depth layer, in October 2014.

The 46 samples (30 from Redenção and 16 from Quixadá) were collected and passed through sieves with a 2 mm mesh opening (maintaining the moisture in which the samples were collected). Subsequently, part of the sample was macerated and passed through a sieve with a 0.2 mm mesh opening. Thus, we analyzed 92 samples, 46 for each particle size (2 and 0.2 mm). We used a portion of approximately 5 g to obtain spectral curves for each of the particle sizes. No other treatment was performed on the samples.

### Obtaining spectral curves and data analysis

We obtained spectral data in the near-infrared (NIR) region using the Perkin Elmer Frontier NIR/IR equipment, with a diffuse reflectance accessory, in the 900–2,500 nm range, resolution 16 cm<sup>-1</sup>, with an average of 32 scans. A total of 4,005 variables (wavelengths) were measured. We used The Unscrambler 10.4X program (CAMO SOFTWARE AS, 2019) for pretreatment of spectral data and the principal component analysis (PCA) as an exploratory method.

Based on the spectral interpretation (Figure 2), we selected wavelengths that have more chemical information of the soil, choosing the 1,360–2,260 nm range (Figure 2), for this is the region of the spectrum that has well-defined absorption bands and no negative influence of instrumental noise. Thus, we used the selected range for the study of pretreatments, PCA and projection classification, considering 2,376 variables.

We evaluated three pretreatments of spectral data: multiplicative scatter correction (MSC), first derivative, and second derivative using the Savitzky-Golay algorithm, with second-order polynomial and a 7-point window.

We used the 1,360–2,260 nm region of spectral bands to verify whether the PCA has the potential to predict the characterization of the soils of the studied locations. For this, we divided the group of samples according to the particle sizes, using the 46 soil samples that passed through the sieve with a mesh opening of 2 mm to build the PCA

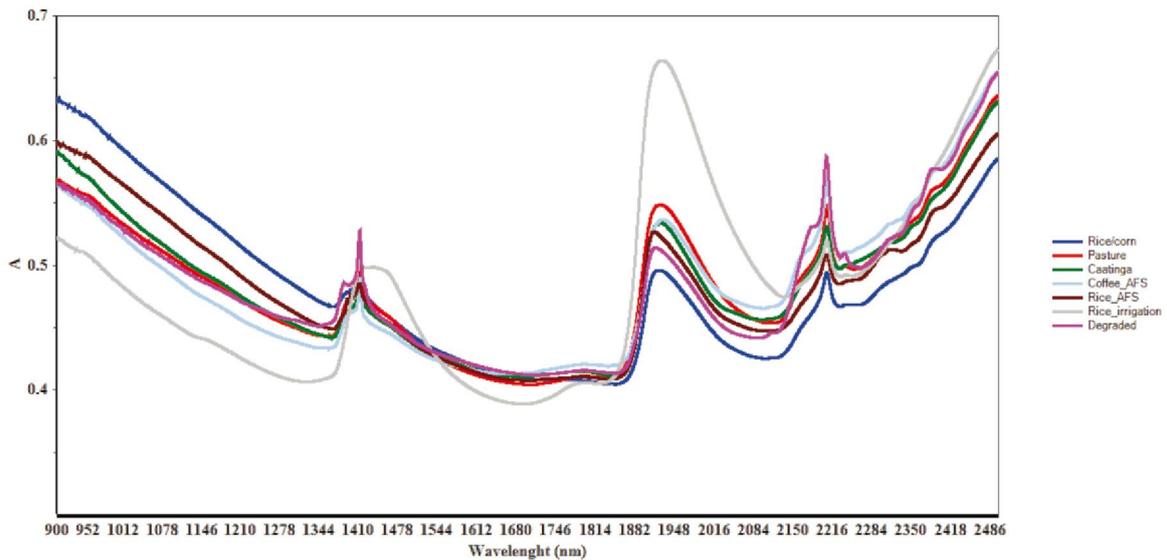
model, as well as the 46 soil samples that passed through the sieve with an opening of 0.2 mm, for predicting the PCA projection (model validation).

## RESULT AND DISCUSSION

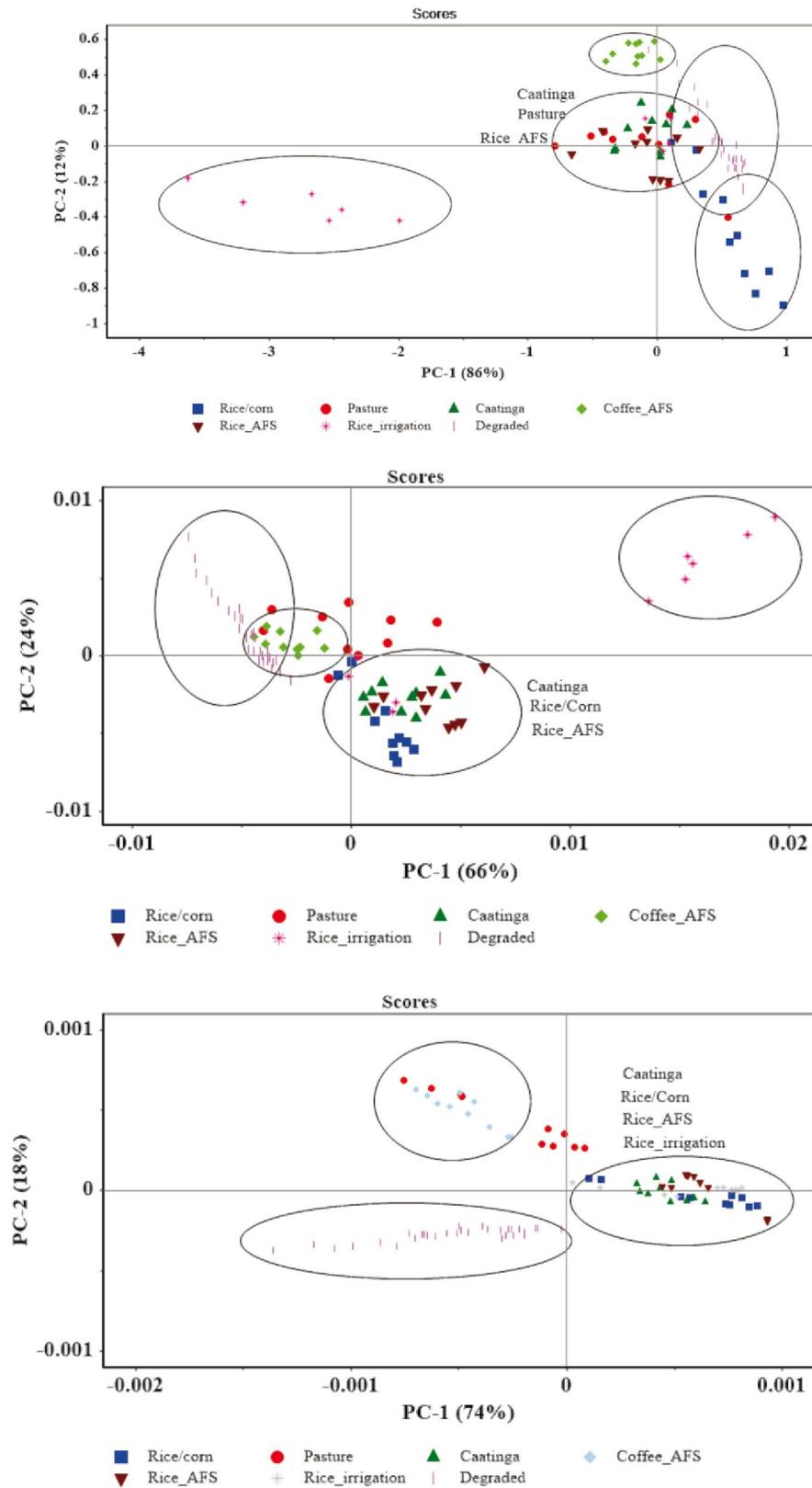
The MSC was the pretreatment with the best result (Figure 3A) because there was a better correlation of spectral data, defining a greater number of classes of soil types according to the management, with highlights for the areas of irrigated rice\_AFS, rice and corn, degraded soil, and coffee\_AFS. The Caatinga, pasture, and rice\_AFS soils showed no significant difference influenced by the main components defined (Figure 3A). On the other hand, the pretreatments of first and second derivatives allowed to form fewer patterns (Figures 3B and 3C). In addition, the first two main components of the MSC contain 98% of the data variability (Figure 3A), while the first and second derivatives pretreatments have less explanation, with 90% and 92% of the data variability, respectively (Figure 3B and 3C).

Figure 4 shows the spectral curves of the soils in each management and particle size (2 mm and 0.2 mm) studied after the multiplicative scatter correction (MSC) pretreatment and in the spectral range with higher absorption values (1,360–1,260 nm) with the interpretation of the absorption bands. It is possible to verify the similarity of behavior of both particle sizes in

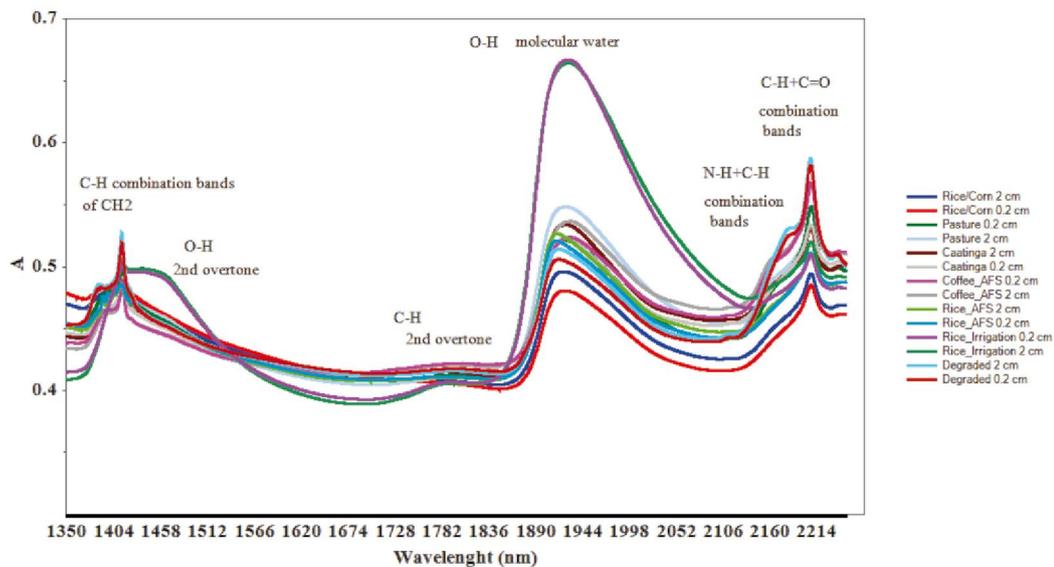
**Figure 2** - Soil spectra under different uses in the 900–2,500 nm region, in Redenção and Quixadá, Ceará State



**Figure 3** - Soil principal component analysis under different uses with spectral data pretreatments: A) multiplicative scatter correction (MSC); B) first derivative Savitzky-Golay; C) second derivative Savitzky-Golay, in Redenção and Quixadá, Ceará State



**Figure 4** - Soil spectra under different uses, with MSC pretreatment in the 0.2 mm and 2 mm particle sizes, in Redenção and Quixadá, Ceará State



practically the entire spectrum regarding the intensity of absorption and position of the peaks. In this sense, Felix *et al.* (2016), observed that the reduction in particle size, despite increasing the absorption intensity of the samples, did not alter the positions of the absorption peaks in the spectrum. Due to the similarity of the spectral profiles of the same sample, but with different particle sizes, the spectral data were treated as a replica of the same soil type, which increases the number of study samples.

Interpretation of the bands according to Viscarra Rossel and Chen (2011), Clark *et al.* (1990), Sheperd and Walsh (2002) and Workman Junior and Weyer (2012).

The absorption bands were in the same regions, with a more pronounced difference in the regions of 1,400 nm and 1,950 nm (Figure 4). The soil of the irrigated rice area in the agroforestry system presented the highest absorptions, while the soil under degraded conditions presented the lowest absorptions (Figure 4). Possibly the largest differences between these two areas, highlighted in the spectral regions mentioned (1,400 nm and 1,950 nm), are related to the chemical bonds of the C–H and O–H groups that present absorption bands close to these regions of the spectrum.

In all evaluated areas, we observed absorption peaks in three distinct ranges, and these peaks are associated with absorption bands present in spectral regions ranging from 1,385 nm to 1,450 nm, from 1,780 nm to 1,930 nm, and from 2,180 to 2,220 nm (Figure 4). Probably, the peaks presented in the first range are related to the chemical bonds of the C–H stretching and deformation combination

groups of CH<sub>2</sub> and CH<sub>3</sub> groups plus O–H associated with the carbon chain (VISCARRA ROSSEL; CHEN, 2011; WORKMAN JUNIOR; WEYER, 2012).

The second range of higher spectral absorptions observed in this study (1,780–1,930 nm) expresses second overtone bands of the C–H group plus the O–H group associated with molecular water (CLARK *et al.*, 1990; SHEPHERD, WALSH, 2002; WORKMAN JUNIOR; WEYER, 2012). The last band presented in the evaluated spectra (highlighted in the 2,180–2,220 nm range) is related to the combination bands of groups N–H, C–H, and C=O, as well as C=O bands of peptide groups (WORKMAN JUNIOR; WEYER, 2012).

Felix *et al.* (2016), also observed absorption peaks in regions close to those observed in the present study, in addition to another band in the region close to 2,400 nm. Similarly, Xu *et al.* (2018) observed absorption peaks in the spectral regions of 1,400 nm, 1,900 nm, and 2,200 nm, with small differences in the shapes of the spectra that indicate subtle absorption peaks for the last band (2,200 nm).

Low-intensity absorption peaks (with subtle absorptions) may represent masked spectral characteristics because measurements are affected by soil roughness, texture, and moisture (XU *et al.*, 2018). Spectral absorption peaks in the bands present in the first and second regions observed in this study (1,385–1,450 nm and 1,780–1,930 nm) may be related to the moisture of the samples (FELIX *et al.*, 2016). Bands located near 2,200 nm are associated with the presence of minerals 1:1 and 2:1 (DEMATTÊ *et al.*, 2015).

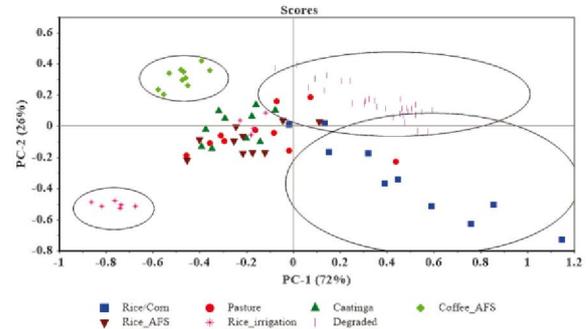
The principal component analysis (PCA) with spectral data pre-treated by MSC (Figure 5) had an explanation of 98% of the data with the first two main components (PC1 and PC2). PC1 explained 72%, and PC2 explained 26% of the total variance. The PCA allowed the identification of five regions that present similar spectral profile patterns, due to the proximity of the points in the PCA projection.

Thus, we differentiated the cultivation area (rice and corn), located on the right side of PC1 and below PC2; the AFS with irrigated rice, with spots located on the left side of PC1 and below PC2; the AFS with coffee, on the left side of PC1 and above PC2; the soil under degradation process, located on the left side of PC1 and above PC2; and the fifth group, formed by samples from the other areas (Caatinga, pasture, and AFS with dryland rice), which formed a large group positioned near the axis of PC1 and PC2 (Figure 5).

The graph of loading as a function of wavelength (Figure 6) indicates the regions of the spectrum that had a greater influence on the formation of the first two main components presented in Figure 5. We observed that the first main component (PC1) is related to the characteristic band of moisture, corresponding to the O–H bond associated with molecular water (FRANCESCHINI *et al.*, 2013; HONG *et al.*, 2019; TERRA; DEMATTE; VISCARRA ROSSEL, 2015).

In Figure 6, it is possible to perceive negative values in the region of 1,930 nm (in the absorption band referring to O–H associated with moisture). This means

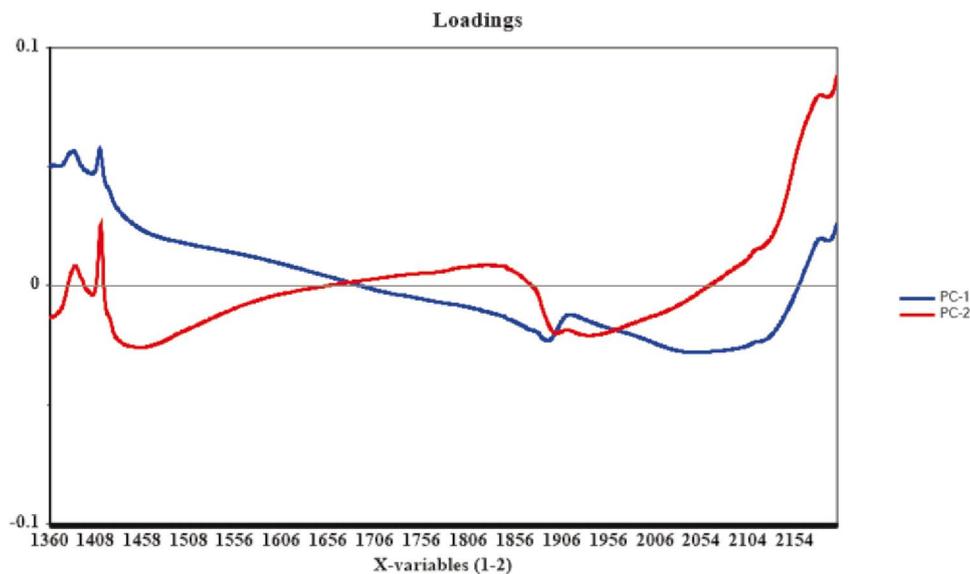
**Figure 5** - Principal component analysis of soils under different uses with pretreatment (MSC), in Redenção and Quixadá, Ceará State



that the samples that have higher moisture values are in the quadrant of the negative values of PC1, especially the areas of AFS with irrigated rice and AFS with coffee (Figure 5). On the other hand, the lower moisture values are in the axis of the positive values, with emphasis, in this region, on soils under rice and corn intercropping and degraded soil (Figure 5).

Other authors support the results presented attributing the highest absorptions in the 1,900 nm region to the vibrations of the O–H radical, present in water molecules (FRANCESCHINI *et al.*, 2013; HONG *et al.*, 2019; TERRA; DEMATTE; VISCARRA ROSSEL, 2015). Felix *et al.* (2016) point out that in soil spectra,

**Figure 6** - Wavelength loadings for the formation of the first two main components (PC1 and PC2) of soils under different uses with pretreatment (MSC), in Redenção and Quixadá, Ceará State



even after drying (in the sample preparation stage), small variations in moisture may be related to absorption peaks between 1,850 nm and 2,030 nm.

The higher moisture level in the AFS areas of irrigated rice and coffee reflects the management with water supply by irrigation in the first area (irrigated rice AFS) and, possibly, the better soil structuring in the coffee AFS, which allows greater water retention in the soil for longer.

The second main component (PC2) is related to the amount of total organic matter derived from the C–H, C=O, and N–H bonds and was evidenced in the bands of the wavelength regions 1,415 nm, 2,184 nm, and 2,208 nm (Figure 6). Thus, soil samples with more information at 1,415 nm are located on the negative side of PC2, especially irrigated rice AFS (Figure 5), while samples with more information at 2,184 nm and 2,208 nm (coffee AFS) are located on the positive axis of PC2 (Figure 5). In this way, the position of the soil samples in relation to this axis may be related not only to the quantity, but also to the composition of organic matter present in soils under the different managements.

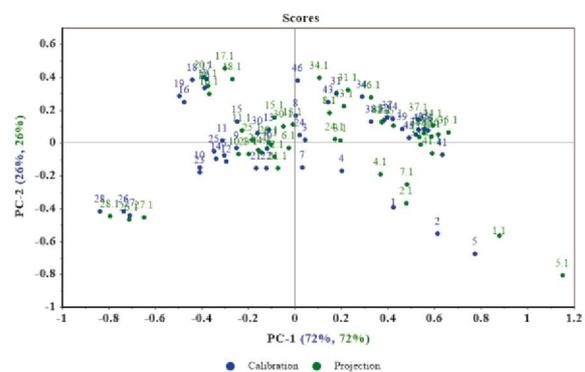
Due to its position in the PCA scatter diagram (Figure 5), we can see that the group formed by the soils in the pasture areas, dryland rice cultivated in the agroforestry system (AFS rice), and Caatinga present intermediate values of moisture and organic matter. The soil in the process of degradation (degraded) has low values of moisture and organic matter; and the traditional intercropping area (rice and corn) presents the lowest moisture values and average organic matter values (Figure 5).

The potential of PCA to demonstrate the different soil characterizations is highlighted by authors such as Dotto *et al.* (2018), and Franceschini *et al.*, (2013). It is likely that these spectral patterns, which allowed distinguishing the groups, are a reflection of the management imposed in the areas, supporting the potential of agroforestry systems (ASF) in maintaining soil quality (AGUIAR *et al.*, 2014; FIALHO *et al.*, 2013). In this study, the rice AFS area presented similar patterns to that of the Caatinga, while irrigated rice AFS and coffee AFS promoted improvements in soil attributes evidenced by moisture and organic matter. On the other hand, traditional managements (rice and corn and degraded area) presented lower moisture and organic matter, as also observed by Fialho *et al.*, (2013).

The PCA modeling of the 2 mm particle size samples and the prediction of the 0.2 mm samples showed a 100% accuracy in the pattern recognition since the samples with different particle sizes were

spatially projected in practically the same positions (Figure 7). This reinforces the understanding that samples of the same soil with different particle sizes present the same spectral profile because, if they had relevant differences, they would have their positions with greater dispersion in the PCA scatter diagram (Figure 7). Thus, the patterns revealed in this analysis with the calibration of the PCA model reinforce the formation of the different groups of soils observed in Figure 5, evidenced by the soil moisture and organic matter factors, as discussed earlier.

**Figure 7** - Principal component analysis of soils under different uses with projection of test samples, in Redenção and Quixadá, Ceará State



## CONCLUSIONS

1. The NIR spectroscopy associated with the data processing methods allowed us to identify distinct spectral patterns for soils under different managements in the regions of the Baturité Massif and the Central Hinterland, Ceará State, thus allowing us to identify soil attributes in these regions;
2. There was no influence of the particle size of soil samples on the spectral response of soils under the different managements evaluated in this study.

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