

NON-DESTRUCTIVE ASSESSMENT OF SOIL ORGANIC CARBON USING NEAR INFRARED TECHNOLOGY

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Abstract

Soil organic carbon (C-organic) is a major component of soil quality that influences the composition of organic materials and the properties of soil mixtures. This C-organic has a practical value and importance in agriculture as well. Normally, conventional and timeconsuming procedures were used to determine C-organic. However, this method is costly, time consuming, involves chemical materials, and may result in pollution. As a result, an alternative fast and environmentally friendly method for determining C-organic in soil is required. The near infrared reflectance spectroscopy (NIRS) technique can be considered for use because it is quick, non-destructive, requires little preparation, and produces no pollution. As a result, the primary goal of this research is to use the NIRS technique to predict C-organics and classify soils based on geographical characteristics. Soil samples were collected from four different site locations, and spectra data were collected in the range of 4000-10 000 cm-1. NIR spectra data and partial least square regression (PLSR) were used to create a C-organic prediction model, while principal component analysis was used to create a classification model (PCA). The results demonstrated that the NIRS technique could predict C-organic with a maximum correlation coefficient (r) of 0.96 and a residual predictive deviation (RPD) index of 4.05, indicating excellent prediction model performance. It is possible to conclude that the NIRS technique can be used to predict C-organic and classify soil characteristics in a quick and non-destructive manner.

Keywords: NIRS, Technology, Agriculture, Soil, Carbon.

Regardless of whether they are food crops or plantations, soil is the most critical substrate for growing plants. In order for plants to thrive, their physical and chemical qualities must be in harmony with those of the soil. The texture, structure, and humidity of the soil can all be used to determine whether or not it is in good health. The amount of nutrients plants need varies based on the stage of growth and the chemical qualities of the soil (Santos et al., 2020). The presence of nutrients in the soil, including macronutrients, secondary nutrients, and micronutrients, has a significant impact on soil fertility. If the soil is low in nutrients, plant growth will be hindered (Johnson et al., 2019). Because soil nutrients do not meet the minimum requirements, growth rate will be disrupted and susceptible to disease. Excess nutrients in the soil, on the other hand, will have an impact on plant growth and the surrounding environment (Afriyie et al., 2022; Wang et al., 2021). Since plants don't utilize artificial nutrient deposits, excessive fertilization and fertilizer use can contaminate the environment, especially in precision agriculture. New difficulties will be compounded by the overuse of pesticides and fertilizers as well as the pollution that results from this. Precision agriculture relies heavily on the organic carbon content (SOC, sometimes referred to as COC) of soils to make it possible (Dong et al., 2021; Santos et al., 2020).

Certainty and precision in determining SOC and soil fraction is essential because it will determine the fertilization dose and application of the correct fertilizer to guarantee that soil has enough nutrients (Peng et al., 2016). Soil texture and nutrient availability can be improved by increasing organic carbon levels in agriculture. The soil fraction, on the other hand, has an impact on plant development and groundwater storage capacity. As a result, gaining an understanding of organic carbon and soil fraction will aid in the selection of plants suitable for present environmental circumstances in precision agriculture or precision farming operations (Darusman et al., 2019; Yunus et al., 2019). In addition, the most effective methods of fertilization and watering will be identified. The fundamental problem that the community is dealing with is the inability to swiftly and in real time predict the organic carbon content and soil fractions.

Soil conditions must be recognized immediately so that plants can grow properly, which demands lengthy laboratory testing. Traditional laboratory testing, on the other hand, necessitates the use of chemicals and pollutes the environment, making it difficult to do (Munawar et al., 2016). To determine the quality parameters of sol carbon organics and other soil characteristics, alternative fast, robust, non-destructive, and pollution-free methods are required. Near infrared reflectance spectroscopy (NIRS) has been developed and widely used in a variety of fields, including agriculture and soil science (Kusumiyati et al., 2022; Munawar, Devianti, et al., 2022; Munawar, Meilina, et al., 2022). Previous research has shown that NIRS can be used in agriculture to determine inner quality parameters, such as in intact fruits (Lan et al., 2020), intact cocoa beans (Hayati et al., 2021; Zulfahrizal & Munawar, 2021), herbal plants (Adib & Abdullah, 2018), biofuels and oil samples (Ambat et al., 2018; Veses et al., 2018), and feed nutritive attributes prediction (Berzaghi et al., 2021). The near infrared reflectance spectroscopy (NIRS) method is based on the idea that biological objects interact with

electromagnetic radiation. Because of this, it is thought to be good for figuring out soil nutrients and other related properties, such as carbon organic. This method has many benefits: it's easy to get a sample ready, it doesn't damage anything, it doesn't make any chemical waste, it doesn't pollute, and it can analyze a lot of samples at once. The results of many studies on how near infrared spectroscopy (NIRS) can be used show that NIRS can be used as a fast, non-destructive tool to predict quality attributes in agricultural sectors (Nicolaï et al., 2007).

The prediction model performance was sufficiently robust and accurate, with correlation coefficients (r) ranging from 0.93 to 0.99 and residual predictive deviation (RPD) indexes ranging from 1.53 to 4.68, indicating coarse, sufficient, and excellent prediction models. We attempted to apply the NIRS method in predicting soil quality parameters in the form of Corganic or SOC based on the advantages and excellence of NIRS as a new, fast, simultaneous, and robust method to determine agricultural and food qualities. Using the partial least square regression (PLSR) method, prediction models were created using the soil spectrum near infrared. The obtained results were then compared to actual C-organic levels measured using standard laboratory procedures.

Materials and Methods

Soil spectral data

The majority of soil samples were collected from four different site locations in Banda Aceh and Aceh Besar and stored for two days to equilibrate before spectral acquisition and further chemical analysis. All soil samples were subjected to near-infrared spectral analysis in the form of a diffuse reflectance spectrum using an infrared instrument (FT-NIR, Thermo Nicolet Antaris II MDS). As a basic measurement in high resolution format, the basic measurement with probe detector was chosen. The infrared spectrum was collected and recorded in wavenumbers ranging from 4000 to 10 000 cm^{-1} , with 32 scans co-added and averaged. Spectra data were saved in three different file formats (*.SPA, *.JDX, and *.CSV) on a local computer (Munawar et al., 2020) .

Detection of Outliers

Outliers in the samples were examined by plotting all spectral data onto principal component analysis and subjecting it to the Hotelling T2 ellipse. Outliers were identified and deleted for data points that fell outside of this ellipse. This procedure was repeated until no more outliers were found. Thus, after removing outliers, the remaining samples were used to build calibration models with different spectra pre-processing (Pasquini, 2018).

Determination of actual organic carbon

Following the completion of the spectra collection, all soil samples were taken immediately to measure soil organic carbon (SOC) or C-organic using an elemental analyzer and a thermal conductivity detector (Santos et al., 2020). Soil organic carbon was expressed as a percentage of total SOC. Actual organic carbon data were measured in triplicate and averaged.

Corrections to NIR spectral data

Near infrared spectra data from soil samples were enhanced and corrected using the following methods: de-trending (DT), multiplicative scatter correction (MSC), and a combination of the two (DT+MSC).

Models of SOC prediction

Prediction models were established and developed to predict SOC or C-organic of soil samples using original untreated spectra data (defined as raw spectrum) and enhanced spectra data (DT, MSC, and combination of DT+MSC). Regressing spectral data (X-variable) and actual Corganic data yielded prediction models (Y-variable). In developing C-organic prediction models, partial least square regression (PLSR) was used as a regression method. The accuracy and robustness of soil organic prediction performances were assessed using several statistical indicators, including coefficient of determination (R2), correlation coefficient (r), root mean square error (RMSE), and residual predictive deviation (RPD), which is defined as the ratio of the standard deviation to the root mean square error. The greater the RPD, the better and more robust the model for predicting C organic of soil samples.

It goes without saying that a good model should have a high R^2 and r coefficient, a low RMSE value, and a small number of PLSR latent variables. High R^2 , r coefficients (equal to or greater than 0.8) and low RMSE are required for good and excellent prediction model performance (Jaconi et al., 2019; Sepúlveda et al., 2021). The RPD, defined as the ratio between the standard deviation of the reference or actual value of SOC and the RMSEP, is another statistical parameter commonly used to interpret and compare NIR calibration models. The higher the value of RPD, the more likely the model is to correctly predict the desired chemical constituent in accurately set samples. The number of factors or latent variables was also considered because they could represent the main characteristics of the spectra, reduce the number of variables, and express the majority of the variance in the data set. To avoid modelling noise signals, fewer latent variables are preferred.

Results and Discussion

Figure 1 depicts a typical diffuse reflectance spectrum for soil samples. It shows several peaks that represent the vibration of C-C, O-H, N-H, C-H-O, and C-H molecular bonds. Before correction, the original spectra data were still contaminated by noise caused by light scattering. These noises were corrected using a combination of pre-treatment methods, including detrending (DT), multiplicative scatter correction (MSC), and DT+MSC. As shown in Fig. 2, these spectral correction methods clearly improve spectral appearance and remove some light scattering noise.

Fig.1 - Typical diffuse reflectance spectra data of soil samples before correction.

Spectral data from a near infrared instrument typically contain background information and noises that interfere with and affect desired relevant soil quality information such as Corganic. Light scattering, path length variations, and random noise caused by variable physical sample properties or instrumental effects must be removed or minimized in order to obtain accurate, robust, and stable calibration models. As a result, it is critical to pre-process spectral data prior to developing a prediction model for C-organic. Spectra data were corrected and enhanced using DT, MSC, and a combination of DT+MSC, as shown in Figure 2. De-trending pre-treatment removes nonlinear trends in spectroscopic data, whereas MSC reduces amplification due to light scattering and offset due to additive chemical effects in near infrared spectra.

Fig. 2 - Near diffuse reflectance spectra after correction using DT, MSC and combination DT+MSC

Following the completion of spectra pre-processing, we developed prediction models for predicting C-organic on soil samples. Partial least squares regression (PLSR) models were developed using untreated and treated spectra from soil samples with wavenumbers ranging from 4000 to 10 000 cm⁻¹. We compared the correlation coefficient (r) , standard error prediction (RMSE), and residual predictive deviation (RPD) indices. The relationship between the observed response variable y (Y-variables: soil C-organic) and the independent variable x constitutes the C-organic prediction model (X-variables: diffuse near infrared reflectance spectrum). The interaction of near-infrared radiation with a biological object yields primary information about its physical, optical, and chemical properties. Table 1 displays the prediction result for soil C-organic.

DT	0.80	0.90	0.21	2.70
MSC	0.86	0.93	0.18	\sim 3.13
DT+MSC	0.93	0.96	0.14	4.05

DT: de-trending, MSC: multiplicative scatter correction, RMSE: root mean square error; R2: determination coefficient, r: correlation coefficient, RPD: ratio prediction to deviation.

To begin, a C-organic (SOC) prediction model was created using unprocessed raw spectra data. It obtained a correlation coefficient of 0.87, an RMSE value of 0.28, and an RPD index of 1.73. When a prediction model was built using DT spectra data, the correlation coefficient increased to 0.90, the RMSE error prediction was reduced to 0.21, and the RPD index was clearly better than before. Furthermore, when the prediction model was developed using MSC spectra data, the accuracy and robustness of the C-organic prediction model were significantly improved. It obtained $r = 0.93$ with RPD = 3.15 and an error of 0.18. Finally, a C-organic prediction model was developed using DT+MSC spectra data to achieve the most accurate and robust prediction result with the highest correlation coefficient $r = 0.96$ and RPD index = 4.05 with the lowest error RMSE $= 0.14$. Figure 3 depicts a scatter plot derived from actual C-organic versus predicted C-organic.

Fig. 3 - Scatter plot between actual and predicted SOC of soil samples using different spectral data (raw, DT, MSC, and DT+MSC).

Furthermore, based on the literature, an RPD index between 1.0 and 1.5 indicates that prediction performance is still coarse and needs to be improved, particularly in terms of spectral data correction. Then, an RPD value between 1.5 and 2.5 indicates that prediction performance is categorized as adequate. Furthermore, RPD values between 2.5 and 3 are classified as good prediction, while RPD values above 3 indicate excellent accuracy prediction performance. When SOC prediction models were built using treated and enhanced spectral data, prediction performance improved significantly. When compared to the raw uncorrected spectra, all spectral correction methods produced higher accuracy and robustness indexes (raw). Furthermore, a hybrid combination of enhanced spectra data, as used in this study with DT and MSC spectra correction methods, was discovered to be the best spectral data from which prediction accuracy reached the maximum correlation coefficient between reference SOC and predicted SOC. As a result, it is obvious that improved spectra would improve prediction accuracy and robustness. Based on the prediction performances obtained from all spectra data, it appears that infrared technology has the potential and capability of predicting SOC content of soil samples with a maximum correlation coefficient of 0.96 and RPD index of 4.05. Furthermore, when the spectra data is corrected and enhanced using a proper correction method, this technology can provide more accurate and robust prediction results.

Conclusion

Based on the findings, we can conclude that near infrared spectroscopy can be used and employed as a quick and environmentally friendly method for predicting soil organic carbon (C-organic). De-trending (DT) and multiplicative scatter correction (MSC) improved prediction accuracy and robustness by increasing the correlation coefficient between actual and predicted C-organic, increasing the RPD index, and lowering the RMSE error prediction. The combination of DT+MSC spectra correction yields the most accurate and robust C-organic prediction result, with $r = 0.96$ and RPD = 4.05.

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