

RAPID AND NON-DESTRUCTIVE PREDICTION OF C-ORGANIC IN AGRICULTURAL SOIL USING NEAR INFRARED REFLECTANCE SPECTROSCOPY (NIRS)

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Abstract. Soil organic carbon (C-organic) is one of main of soil quality which affects the assortment of organic materials and mixtures properties of soils. This C-organic also have a practical value and importance in agriculture. To determine C-organic, normally, conventional and laborious procedures were employed. Yet, this method is expensive, time consuming, involve chemical materials and may cause pollution. Thus, alternative fast and environmental friendly method is required to determine C-organic in soil. The near infrared reflectance spectroscopy (NIRS) technique can be considered to be applied, since this method is fast, non-destructive, simple preparation and pollution free. Therefore, the main objective of this present study is apply NIRS technique in predicting C-organics and classifying soils based on geographical characteristics. Soil samples from 4 different site locations were taken spectra data of these samples were acquired in wavenumbers range of 4000-10 000 cm^{-1} . C-organic prediction model was developed using NIR spectra data and partial least square regression (PLS), while classification model was established using principal component analysis (PCA). The results showed that Soil characteristics from 4 different locations can be classified with total explained variance of PCA was 99% (PC1 = 88% and PC2 = 11%). Moreover, NIRS technique was able to predict C-organic with maximum correlation coefficient (r) was 0.93 and residual predictive deviation (RPD) index was 3.22 which categorized as excellent prediction model performance. It may conclude that NIRS technique can be applied as a rapid and non-destructive method in predicting C-organic and classifying soil characteristics.

1. Introduction

Soil is the main media for growing plants, whether it is food crops or plantations. In fact, plants can grow ideally on healthy soil, if the soil has physical and chemical properties that are suitable with plant growth. Healthy soil conditions can be seen visually by looking its texture, structure and humidity. Soil chemical properties are related to the amount of nutrients needed by plants, with the amount needed will be different for each growing phase [1]. Soil fertility is largely determined by the presence of nutrients in the soil, both macro nutrients, secondary, and micro nutrients. Nutrients that are lacking in the soil will obviously affect plant growth. Growth rate will be very disturbed and susceptible to disease

because soil nutrients do not meet the minimum requirements needed. Conversely, the amount of excessive nutrients in the soil will also affect plant growth and the surrounding environment [2].

In precision agriculture practice, fertilization and excessive use of fertilizer will cause pollution to the environment because it can cause artificial nutrient deposits that are not utilized by plants. This of course will accumulate and make new problems especially pollution due to the use of pesticides, fertilizers and fertilizers that are above the normal amount [3].

Carbon organic or sometimes called as organic carbon content (SOC), is one of main soil characteristics that play an important role in precision agriculture practice. The amount of SOC and soil fraction must be known certainly and precisely, because it will determine the fertilization dose and the use of the right fertilizer so that the optimum amount of nutrients in the soil is sufficient [1, 2]. Organic carbon levels play an important role in agricultural practices because these factors are able to improve the availability of nutrients, and soil texture. On the other hand, the soil fraction also affects plant growth and ground water storage capacity or water holding capacity. Thus, knowing these two factors (organic carbon and soil fraction) will help in the decision-making process in precision agriculture or precision farming practices, especially for the selection of plants that are suitable for the existing environmental conditions. In addition, this will also determine suitable types of fertilization and irrigation to produce maximum agricultural production.

The main problem faced in the community is the difficulty of predicting organic carbon content and soil fractions quickly and in real time. This requires testing in a laboratory which is time consuming, while the soil conditions must be immediately known so that plants can grow ideally. In addition, conventional testing in the laboratory is also sometimes complicated in the process, requiring chemicals and can cause environmental pollution [4].

Alternative fast, robust, non-destructive and pollution free methods are required to determine quality parameters of soil carbon organics and other soil characteristics. Near infrared reflectance spectroscopy (NIRS) has been developed and widely applied in many sectors including in agriculture and soil science [5].

Near infrared reflectance spectroscopy (NIRS) technique works based on the principle of interaction of electromagnetic radiation with biological objects like soil. This method is potential to be implemented for determining soil nutrients and other related properties including carbon organic. The advantage of this method are: simple sample preparation, non-destructive in nature, no chemical waste, pollution free, simultaneous and high speed of analysis. [5, 6].

The overall research findings of numerous studies on the application of near infrared spectroscopy (NIRS), shows that NIRS was feasible to be applied as a rapid and non-destructive tools for quality attributes prediction in agricultural sectors. The prediction model performance was sufficiently robust and accurate with correlation coefficient (r) range of 0.93 – 0.99 and residual predictive deviation (RPD) index was 1.53 – 4.68 which is categorized as coarse, sufficient and excellent prediction models respectively.

Based on advantages and excellence of NIRS as a new, fast, simultaneous and robust method to determine agricultural and food qualities, we attempted to apply the NIRS method in predicting soil quality parameter in form of C-organic or SOC. Prediction models were established using soil spectrum near infrared using partial least square regression (PLSR) method. Obtained results were then compared to actual C-organic measured by standard laboratory procedures.

2. Materials and Methods

2.1. Samples

A bulk of soil samples from four different site locations in Banda Aceh and Aceh Besar area were taken and stored for two days to equilibrate before spectra acquisition and further chemical analysis.

2.2. Near infrared spectrum acquisition

Infrared spectral data in form of diffuse reflectance spectrum were taken of all soil samples using infrared instrument (FTIR, Thermo Nicolet Antaris II MDS). The basic measurement with probe detector was chosen as a basic measurement in high resolution format. Infrared spectrum were collected and recorded in wavenumbers range from 4000 to 10 000 cm^{-1} with co-added 32 scans and averaged.

Spectra data were stored in local computer with three different file formats (*.SPA, *.JDX and *.CSV) [5].

2.3. C-organic measurement

Once after spectra collection was completed, all soil samples were taken immediately to measure soil organic carbon (SOC) or C-organic using *elemental analyzer* and *thermal conductivity detector*. Soil organic carbon were expressed as % SOC [1]. Actual carbon organic data were measured in triplicate and averaged.

2.4. Spectra data correction

In order to obtain accurate and robust prediction results, infrared spectra data were enhanced and corrected using these following methods: de-trending (DT), multiplicative scatter correction (MSC), and combination of them (DT+MSC) [6].

2.5. C-organic prediction model

Prediction models, used to predict SOC or C-organic of soil samples were established and developed using original untreated spectra data (defined as raw spectrum) and enhanced spectra data (DT, MSC and DT+MSC). Prediction models were established using partial least square regression (PLSR) [5, 7].

2.6. Model evaluation performance

Soil organic prediction performances were evaluated for their accuracies and robustness using several statistical indicators: coefficient of determination (R^2), correlation coefficient (r), root mean square error (RMSE) and the residual predictive deviation (RPD) [5, 6]. It is obvious that the good model should have high R^2 and r coefficient, low value of RMSE and few number latent variables of PLSR [8, 9].

3. Result and discussion

3.1. Typical spectra of soil sample

Typical diffuse reflectance spectrum for soil samples were presented in Fig.1. it shows several peaks represent the vibration of molecular bonds of C-C, O-H, N-H, C-H-O and C-H. Original spectra data before correction were still interference due to noise resulted from light scattering [10, 11]. These noises were corrected using several pre-treatment methods namely de-trending (DT), multiplicative scatter correction (MSC) and combination of them (DT+MSC). As shown in Fig. 2, these spectra correction methods clearly enhance spectra appearance and remove some noises due to light scattering.

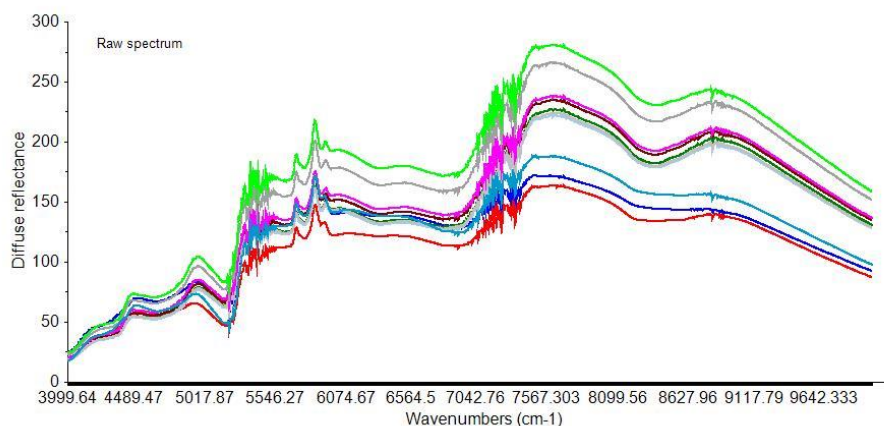


Fig.1. typical diffuse reflectance spectra data of soil samples before correction.

Spectral data acquired from the near infrared instrument generally contain background information and noises which are interfered and affected desired relevant soil quality information such as C-organic. Interfering spectral parameters, such as light scattering, path length variations and random

noise resulted from variable physical sample properties or instrumental effects need to be removed or minimized in order to obtain accurate, robust and stable calibration models. Thus, it is very necessary to pre-process spectral data prior to prediction model development used to predict C-organic.

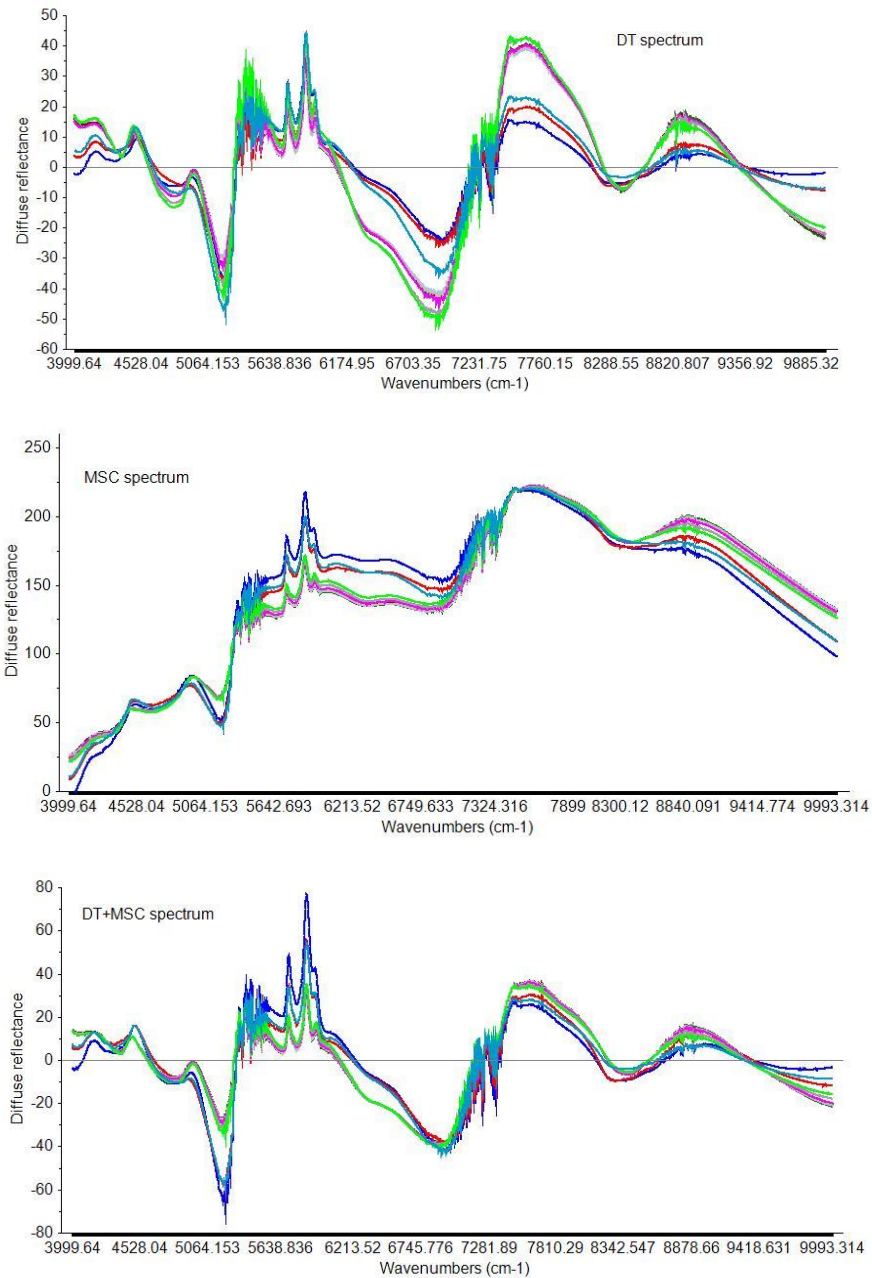


Fig.2. diffuse reflectance spectra after correction using DT, MSC and combination DT+MSC.

As shown in Fig.2, spectra data were corrected and enhanced using DT, MSC and combination of DT+MSC. The de-trending pre-treatment method tends to remove nonlinear trends in spectroscopic data, while MSC method used to reduce amplification due to light scattering and offset due to additive chemical effects in near infrared spectra

3.2. Prediction models

After spectra pre-processing were completed, we established prediction models used to predict C-organic on soil samples. Partial least squares regression (PLSR) models were built based on untreated and treated spectra using soil samples datasets with the wavenumbers range from 4000 – 10 000 cm^{-1} . The correlation coefficient (r), standard error prediction (RMSE) and residual predictive deviation (RPD) index, were compared.

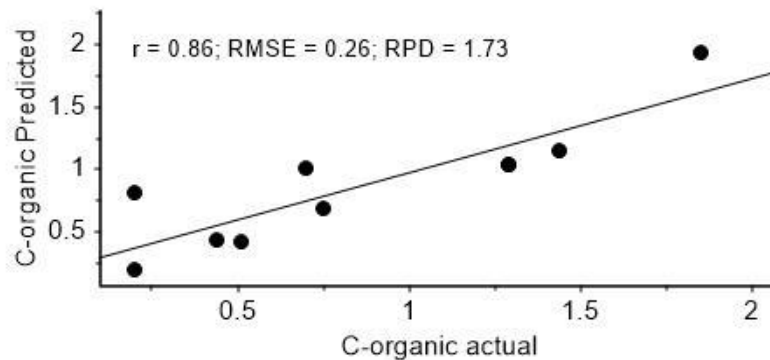
C-organic prediction model consists of the relationship between the observed response variable y (Y-variables: soil C-organic) and the independent variable x (X-variables: diffuse near infrared reflectance spectrum). The primary information that can be gathered from the interaction of the near-infrared radiation with the biological object is its physical, optical and chemical properties. Prediction result for soil C-organic was shown in Table 1.

Table 1. C-organic prediction performance using diffuse reflectance spectra data

Spectrum	Statistical indicator			
	R^2	r	RMSE	RPD
Raw	0.75	0.87	0.26	1.73
DT	0.80	0.90	0.21	2.70
MSC	0.86	0.93	0.18	3.15
DT+MSC	0.93	0.96	0.14	4.05

R^2 : coefficient of determination, r : correlation coefficient, RMSE: root means square error, RPD: residual predictive deviation, DT: de-trending, MSC: multiplicative scatter correction.

Firstly, C-organic prediction model was developed using untreated raw spectra data. It achieved correlation coefficient of 0.87, with RMSE value = 0.28 and RPD index = 1.73. When prediction model was developed using DT spectra data, the correlation coefficient was increased become 0.90 and RMSE error prediction was decreased to 0.21 and RPD index obviously better than previous. Moreover, accuracy and robustness of C-organic prediction model were significantly improved when prediction model was developed using MSC spectra data. It achieved $r = 0.93$ with RPD = 3.15 and error decreased to 0.18. Finally, C-organic prediction model was established using combination DT+MSC spectra data to achieve most accurate and robust prediction result with maximum correlation coefficient $r = 0.96$ and RPD index = 4.05 with lowest error RMSE = 0.14. Scatter plot derived from actual C-organic versus predicted C-organic were presented in Figure 3.



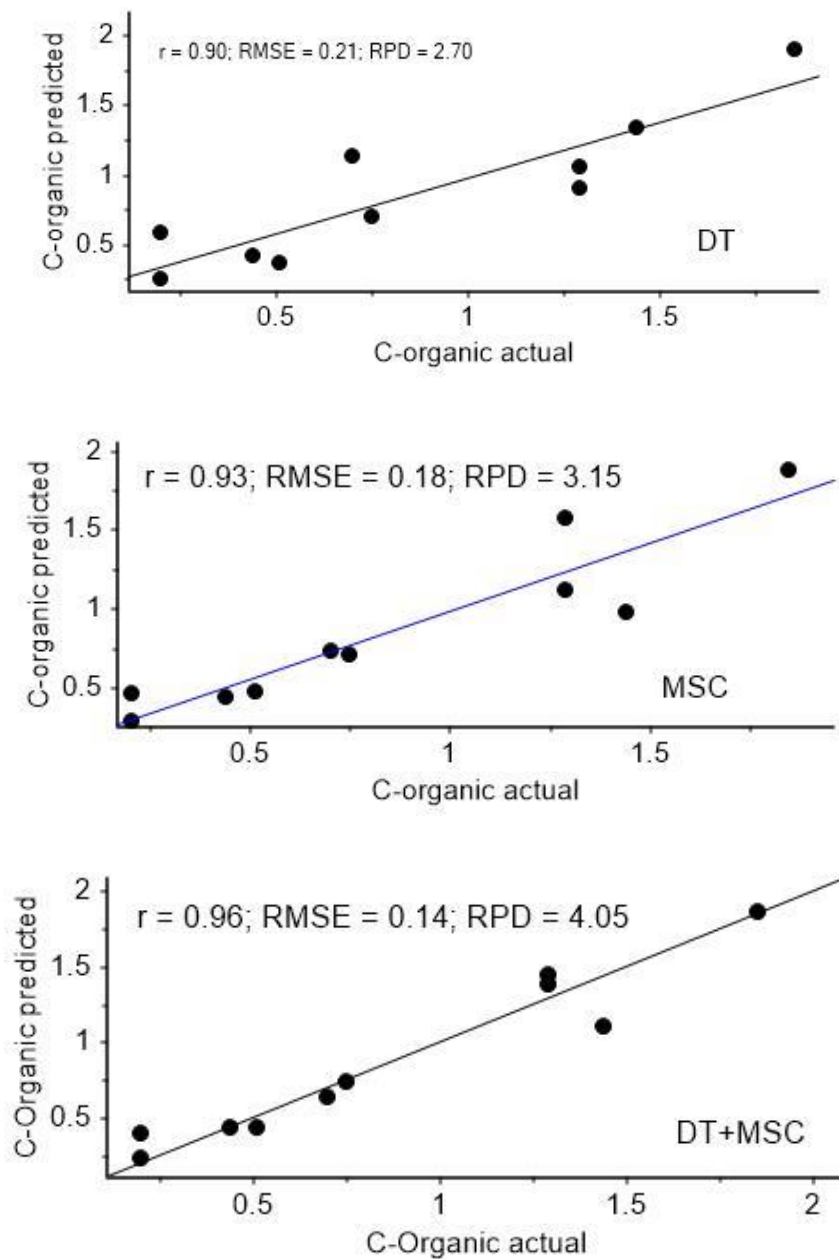


Fig. 3. Scatter plot between actual and predicted C-organic of soil samples using NIR spectra data.

4. Conclusion

Based on obtained results, we may conclude that near infrared spectroscopy can be applied as a rapid alternative method used to predict soil organic carbon (C-organic). Spectra correction using De-trending (DT), multiplicative scatter correction (MSC) were obviously improved prediction accuracy and robustness by increasing correlation coefficient between actual and predicted C-organic, increasing RPD index as well as lowering RMSE error prediction. A combination of DT+MSC spectra correction provide the most accurate and robust C-organic prediction result with correlation coefficient $r = 0.96$ and $RPD = 4.05$.

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