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Fast And Simultaneous Prediction Of Agricultural Soil Nutrients Content Using Infrared Spectroscopy

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Abstract

The functions soil depends on the balances of its structure, nutrients composition as well as other chemical and physical properties. Conventional methods, used to determine nutrients content on agricultural soil were time consuming, complicated sample processing and destructive in nature. Near infrared reflectance spectroscopy (NIRS) has become one of the most promising and used non-destructive methods of analysis in many field areas including in soil science. The main aim of this present study is to apply NIRS in predicting nutrients content of soils in form of total nitrogen (N). Transmittance spectra data were obtained from a total of 18 soil samples from 8 different sites followed by N measurement using standard laboratory method. Principal component regression (PCR) with full cross validation were used to develop and validate N prediction models. The results showed that N content can be predicted very well even with raw spectra data with coefficient correlation (r) and residual predictive deviation index (RPD) were 0.95 and 3.35 respectively. Furthermore, spectra correction clearly enhances and improve prediction accuracy with $r = 0.96$ and $RPD = 3.51$. It may conclude that NIRS can be used as fast and simultaneous method in determining nutrient content of agricultural soils.

Keywords : *infrared; soil; nitrogen; prediction; spectroscopy*

Prediksi Cepat dan Simultan Kandungan Nutrisi Tanah Pertanian Menggunakan Spektroskopi Inframerah

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Abstrak

Fungsi tanah tergantung pada keseimbangan struktur, komposisi hara, serta sifat kimia dan fisik lainnya. Metode konvensional, yang digunakan untuk menentukan kandungan hara pada tanah pertanian memakan waktu, proses sampel yang rumit dan merusak di alam. Near infrared reflektansi spektroskopi (NIRS) telah menjadi salah satu metode analisis non-destruktif yang paling menjanjikan dan digunakan di banyak bidang termasuk dalam ilmu tanah. Tujuan utama dari penelitian ini adalah untuk menerapkan NIRS dalam memprediksi kandungan nutrisi tanah dalam bentuk nitrogen total (N). Data spektra transmisi diperoleh dari total 18 sampel tanah dari 8 lokasi berbeda diikuti oleh pengukuran N menggunakan metode laboratorium standar. Regresi komponen utama (PCR) dengan validasi silang penuh digunakan untuk mengembangkan dan memvalidasi model prediksi N. Hasil penelitian menunjukkan bahwa konten N dapat diprediksi dengan sangat baik bahkan dengan data spektra mentah dengan koefisien korelasi (r) dan indeks deviasi prediktif residual (RPD) masing-masing 0,95 dan 3,35. Selain itu, koreksi spektra jelas meningkatkan dan meningkatkan akurasi prediksi dengan $r = 0,96$ dan $RPD = 3,51$. Dapat disimpulkan bahwa NIRS dapat digunakan sebagai metode cepat dan simultan dalam menentukan kandungan nutrisi tanah pertanian.

Kata Kunci : inframerah; tanah; nitrogen; ramalan; spektroskopi

INTRODUCTION

As all we know that a major function of soil is to provide fundamental natural resources for survival of plants, animals, and the human race. The functions soil depends on the balances of its structure and composition, well as the chemical, biological, and physical properties (T, Shi., et .al, 2014).

The maintenance of soil quality is critical for ensuring the sustainability of the environment and it depends on the balances of soil structure and nutrient contents. These nutrient contents are divided onto macro and micro nutrient content. N, P, and K are major or macro nutrient contents, while Fe, Mn, Zn, Cu, B, Mo and Cl are known as micro nutrient contents. Both macro and micro are essentially required by plants to grow and develop (J. Wang, 2014).

Significantly, plants can grow optimally in a healthy soil, heavy metals free and fertile. Soil chemical properties related to the amount of nutrients required by plants, the amount needed will vary each growth phase.

It is very difficult to determine nutrient contents on soil in real time and without sample preparation. Normally, it requires standard laboratory procedures in which took some time with complicated sample preparation, and followed with multi step procedures. On the other hand, soil nutrient contents must be determined rapidly in order to take an action required and ensure optimum plant growth.

During the last two decades, infrared (IR) spectroscopy has been widely employed as an effective tool for the analysis of soil properties. Compared with traditional wet chemistry analysis, IR analysis is rapid, cost effective, non-destructive, requires minimal sample preparation and can be used in situ. More importantly, it permits a quantitative assessment of several properties from a single measurement. This technique mainly measures overtones and combinations of fundamental vibrational bands for O-H, N-H and C-H bonds from the mid-infrared region.

Numerous studies for the measurement of soil nitrogen (N) and organic carbon (OC) have been reported using this technique (G. Senesi, & Senesi. N, 2016., M.S Askari, et al., 2015., A.M.R. Bieganowski, & Witkowska, B., 2010).

The IR Spectroscopy is a technique or method which uses infrared radiation of the electromagnetic spectrum to analyze the chemical composition of organic matter. It provides information through spectra signatures and patterns, regarding with the intrinsic organic bonds of the molecules and thus the primary chemical constituents of the object can be determined (H. Cen, & He, Y., 2007).

The term spectroscopy is the study of electromagnetic radiation as a function of wavelength, which has been reflected, absorbed or transmitted from a solid, liquid or gas material. Spectroscopy generates a unique spectral pattern of the material monitored. Each biological object has its own special optical properties, which means it has a different spectra pattern or signatures indicated its chemical compositions (B. M. Nicolai, et al., 2007)

The main objective of this study is evaluate the feasibility of infrared spectroscopy technique, in form of near infrared transmittance spectrum for N content prediction on soil samples. Also, this study is aimed to evaluate the impact of spectra correction on prediction accuracy and robustness compared to un-corrected spectra data.

MATERIALS AND METHOD

A. Soil samples and instrument preparation

Soil samples were collected from 8 different sites in Banda Aceh and Aceh Besar district area. They cover rice field, ground/planted field and bare land. Soils amples were taken to the lab, dried and stored for 3 days prior to spectra acquisition and data analysis. Furthermore, FT-IR iptek 1516 was used as infrared instrument to acquire and record transmittance spectra of soil samples.

B. Transmittance near infrared spectra acquisition

In this study, infrared spectra data of all soil samples were acquired in form of transmittance spectral data. Background spectra correction was performed every hour automatically. Transmittance spectra in wavelength range of 1000 – 2500 nm with the increment of 0.2 nm resolution were acquired 32 times, averaged and recorded in SPA and CSV extension files format.

C. Nitrogen content measurement

Once spectra acquisitions were completed, total nitrogen content were measured using standard laboratory method. These data were used as data validation.

D. Spectra data correction

To enhance and improve prediction performance, spectra correction was employed to all spectra data of soil samples. Standard normal variate (SNV) was chosen as spectra data correction method (A.A. Munawar, 2016).

E. N content prediction

Nitrogen content of soil samples were predicted based on transmittance spectra data using principal component regression (PCR). To validate the prediction result, full cross validation was applied during calibration model development. Model performance was quantified using statistical indicators: coefficient determination (R^2), coefficient correlation (r), the root mean square error (RMSE) and residual predictive deviation (RPD) index.

RESULT AND DISCUSSION

Soil spectra spectrum for all 18 soil samples were presented in Fig.1. Soil spectral features in the infrared wavebands are highly correlated to the vibration modes of functional groups like the chemical bond of H and C, N, and O. These bonds are subject to vibrational energy changes in which two vibration patterns exist in these bonds including stretch vibration and bend vibration.

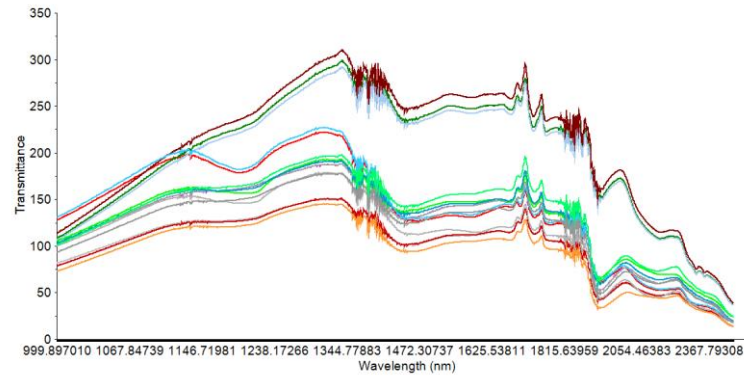


Fig.1. Transmittance spectrum for all 18 soil samples from 8 different sites in Banda Aceh and Aceh Besar.

The nitrogen (N) content in the soil is a macro-element that plays an important role in soil nutrition along with Phosphorus (P) and Kalium (K).

N content prediction, performed using raw un-corrected spectra data was firstly employed to predict N content of soil samples. Prediction result is showed in Fig.2. The accuracy of this prediction is relatively high. It generates correlation coefficient of 0.95 with RPD index of 3.25 which is categorized as excellent model performance.

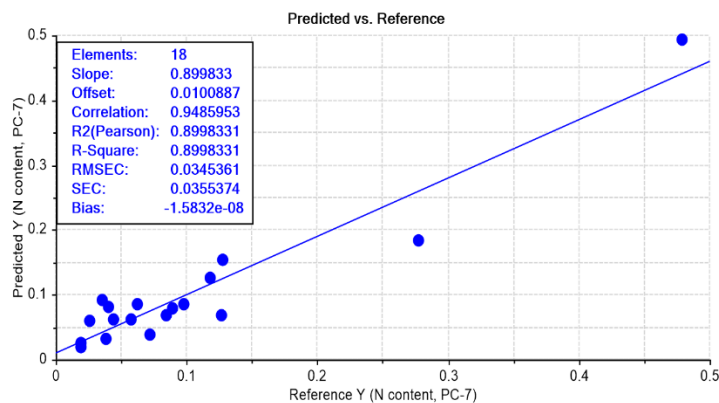


Fig.2. N content prediction result using raw un-corrected transmittance spectra data.

We attempted to correct the spectra data in order to study the impact of this correction on prediction accuracy and robustness. SNV was chosen as a spectra correction method and the prediction result is shown in Fig.3.

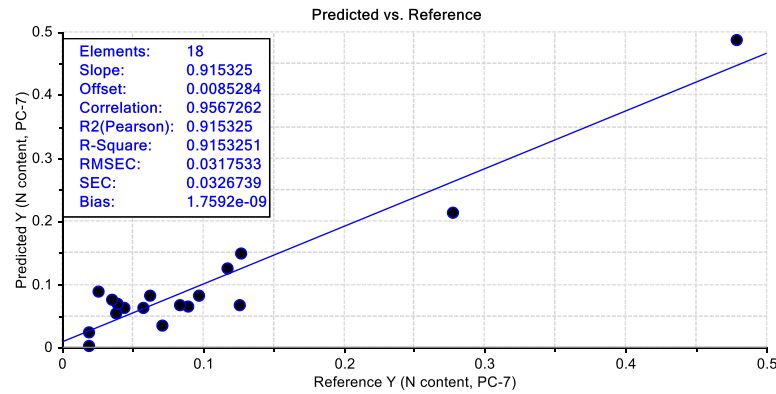


Fig.3. N content prediction result using SNV corrected transmittance spectra data.

Most absorption bands in the infrared region are overtone or combination bands of fundamental absorption bands in the infrared region of the electromagnetic spectrum which are due to vibrational and rotational transitions.

In large molecules and in complex mixtures, such as soil structures, the multiple bands and the effect of peak-broadening result in spectral data that have a broad envelope with few sharp peaks. Soil is the biological object that contains a great quantity of hydrogenous bonds (i.e C-H, O-H and N-H).

Based on this present study, as shown in loading plot in Fig.4, the N content of soil samples can be optimally predicted in wavelength range of 1183 – 1208 nm, and also can be predicted in wavelength range of 1671 – 1753 nm, and 1905 – 1958 nm.

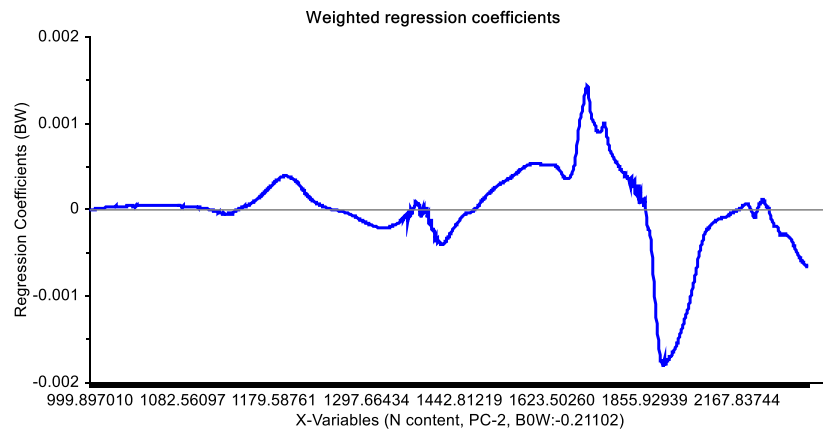


Fig.4. Optimum and relevant wavelength range for N content prediction in NIR region.

CONCLUSION

The present study aimed to evaluate the feasibility of infrared technology as a rapid and non-destructive method in determining soil quality parameter in form of Nitrogen content. Obtained results shows that infrared technology was able to predict N content of soil samples satisfactory with r coefficient = 0.95 and RPD = 3.25. Furthermore, spectra correction, using SNV method was obviously improve prediction accuracy to $r = 0.96$ and RPD index = 3.51.

N content of soil samples can be optimally predicted in wavelength range of 1183 – 1208 nm, and also can be predicted in wavelength range of 1671 – 1753 nm, and 1905 – 1958 nm.

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