



RAPID AND NON-DESTRUCTIVE QUALITY ASSESSMENT OF AGRICULTURAL SOIL USING NEAR INFRARED SPECTROSCOPY

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ABSTRACT

Presented works aimed to apply the near infrared reflectance (NIRS) technology in determining rapidly nitrogen content of agricultural soil. Judging from prediction performances, it seems that NIRS technology can predict the soil nitrogen content in various agricultural land-use and depths. Prediction performance can be improved by establishing models by means of pre-treatments like SNV and BSC methods. The correlation coefficient was improved from 0.71 using raw model, to 0.74 and 0.76 using SNV and BSC spectral data respectively. As a consequence, the prediction error was decreased. In term of ratio prediction to deviation (RPD) index, the model is categorized as sufficient prediction performance and still can be improved by employing hybrid spectra corrections or non-linear regression approach.

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1. INTRODUCTION

Soil chemical characteristics are connected to the quantity of nutrients required by plants, with the amount required varying depending on the growth phase. The presence of nutrients in the soil, both macronutrients, secondary nutrients, and micronutrients, determines soil fertility in major part. Nitrogen (N), phosphorus (P), and potassium (K) are examples of macronutrients (Wang et al., 2021). All plants need macronutrients, particularly during the growth period. The identification of nitrogen, phosphorus, and soil carbon nutrients is critical for determining the amount of fertilizer to be applied to a plant. Nitrogen (N) is an essential element that operates in plants to construct amino acids or proteins, nucleic acids, nucleotides, and chlorophyll, such that in the presence of N, plants become greener, plant

development accelerates, and crop protein content increases. Runoff ranges from 12 to 25 percent, with erosion around 11 percent (Munawar et al., 2020).

Nitrogen in the soil is derived from organic matter in the soil, which is bound by microbes from air N, fertilizers, and precipitation. Elemental N is abundant in the air, accounting for around 78 percent. However, since Air N comes in the form of N₂ gas, it cannot be used directly by plants. Plants can only absorb accessible forms of nitrogen, such as ammonium and nitrate (Dong et al., 2021; Hutengs et al., 2019). As a result, in order for N₂ to be used by plants, it must first be transformed into the bound form of N. The N fixation may be accomplished chemically or biologically via industrial procedures (Singh et al., 2019).



To generate new cells, growing plants need N. Photosynthesis makes carbohydrates from CO₂ and H₂O, but it cannot produce proteins, nucleic acids, and other proteins when N is not present. As a result, severe N shortage will halt the process of development and reproduction. One of the reasons of stunted plants is a lack of N (Cheng et al., 2019; Santos et al., 2020). Plants may absorb excessive levels of nitrogen, particularly when additional factors such as phosphorus, potassium, or a lack of water are present. Many forms of land use may alter soil fertility. Evaluation of soil fertility is a means to diagnose nutrients in the soil. Evaluation of soil fertility is also useful to evaluate the condition of soil fertility in an agricultural area. It is necessary to measure and monitor soil fertility in order to determine the nutritional components that are limiting plant growth (Lazaar et al., 2020). The purpose of determining soil fertility status is to examine soil properties and identify the major impediments to soil fertility. Therefore, the main objective of this presented study is to apply the near infrared (NIRS) technology as a rapid and non-destructive method for N content prediction in agricultural soil. Prediction models were developed based on near infrared spectral data of soil samples by means of principal component regression (PCR) and partial least square regression (PLS) respectively.

2. MATERIALS AND METHODS

2.1. Soil samples

Data inventory is carried out by collecting administrative maps, soil type maps, slope maps and land use maps. The overlay maps were carried out to determine the points of soil sampling so that 11 points of land use unit were obtained. For each site, two soil samples were taken, namely the top layer and the bottom layer until there was a change in the soil. The material used in this study is soil samples from several different locations in the *Aceh Besar* region which only focus on agricultural land (Munawar et al., 2019). All soil samples were then taken to the laboratory to be dried at room temperature for three days to homogenize temperature and humidity before being analysed. Soil samples were ground with mortar and sieved through a 20 mesh (0.84 mm) sieve to remove stones, insects, large debris, gravel, and other unwanted materials. This is done to minimize the effect of

spectral noise due to the influence of soil particle size (Hong et al., 2019)

2.2. Near infrared spectral data

The infrared spectrum for soil samples was collected using the infrared spectroscopy instrument with workflow configuration made using the integrated *Thermo Integration* software[®]. The wavelength range employed is 1000-2500 nm, with a 0.2 nm interval (Devianti et al., 2021). The soil sample was spectroscopically sampled by putting it in a plastic bag. To achieve complete light penetration, the soil sample was put onto a cylindrical quartz dish with a depth of 10 mm. The cylindrical dish was leveled after filling it with 20 g of soil sample. The equipment is programmed to do 32 scans per acquisition at 0.2 nm resolution and 4x optical magnification. To account for variability and density variations, soil samples were put in three cups and spectral measurements were averaged.

2.3. Near infrared spectra data pre-treatments

Before being utilized for further data analysis namely building prediction models, the infrared data spectrum was rectified and enhanced by removing various forms of data spectrum "noises" on the spectrum of soil samples, resulting in more accurate prediction results. Spectrum correction techniques include Baseline Shift Correction (BSC) and Standard Normal Variate (SNV).

2.4. Nitrogen prediction model

The nutrient content of soil samples was predicted using NIR spectrum data (raw). The model calibration phase was followed by cross-validation. The prediction model was created by regressing the spectrum data as the X variable with nutrients and the actual data as the Y variable, i.e. the outcomes of laboratory measurements. Principal Component Regression (PCR) and Partial Least Square Regression (PLSR) are the calibration methods employed at this step (Arendse et al., 2018; Pasquini, 2018). Validation and assessment of the prediction model The developed prediction model will next be evaluated for dependability and accuracy using the k-fold cross validation approach and additional soil samples from other locations. The model's justification accuracy and reliability are based on statistical measures such as the

correlation coefficient (r) between prediction results and laboratory standard measurements, Root Mean Square Error (RMSE), and Residual Predictive Deviation (RPD). A model with high r and RPD parameter values, low RMSE and RMSE difference, and fewer latent variables (LV) is ideally a dependable and accurate predictor model.

3. RESULTS AND DISCUSSIONS

The near infrared reflectance spectrum for soil sample in wavelength range from 1000 to 2500 nm is shown in Fig.1. Radiation-exposed samples Infrared Spectroscopy with wavenumber 1000-2500 nm will receive energy that produces

vibrations and strains in the molecular bond groups of OH, NH, and CH atoms, which are the key components composing organic compounds, and may reveal soil nutrient content owing to the interaction of molecular bonds. Some energy will be absorbed, while some will be reflected. About 4% of the energy released by organic matter is reflected back to the exterior surface (regular reflection), while the other 96 percent enters the substance and experiences absorption, reflection, scattering, and transmission. When radiation strikes a sample, three radiation phenomena occur: absorption (absorbed), transmission (transmitted), and reflection (reflected).

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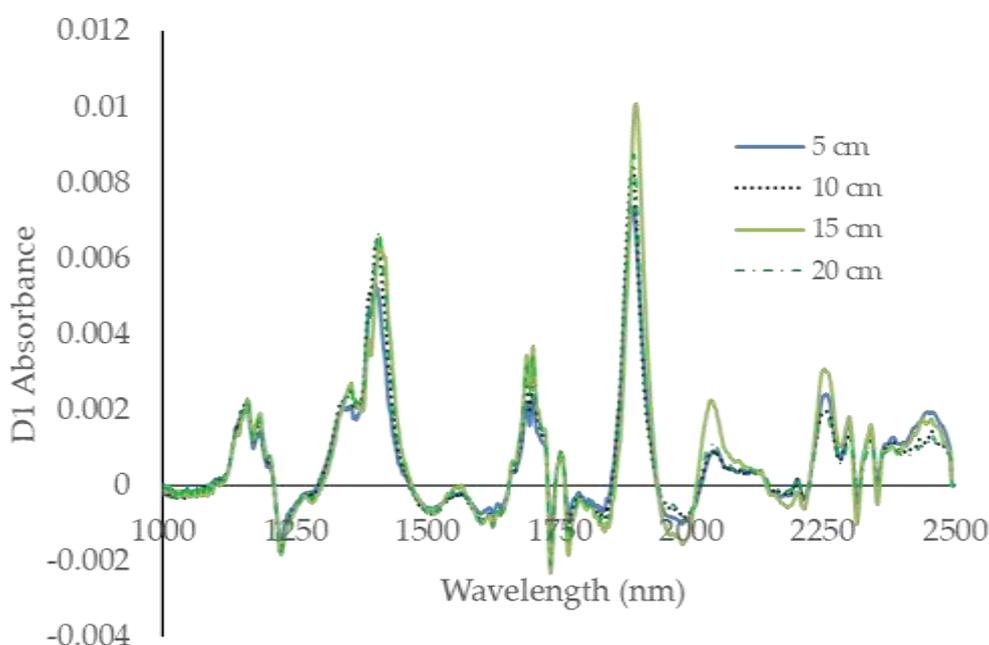


Fig. 1 - Near infrared spectrum of soil samples

The contribution of each phenomena is determined by the sample's chemical composition and physical properties. The contribution of each phenomena is determined by the sample's chemical composition and physical properties. Figure 1 shows the spectrum without improvement. The broad soil NIR spectral pattern may be shown to be almost identical. The smaller the reflected wave, the greater the absorption of the wave. The existence of atomic bonds in the soil at the same infrared wavelengths is shown by the similarity of the soil NIR graph pattern. The distinction is in the amplitudes, which are affected by the concentration of each of these bonds in the soil. The absorption and wave amplitude increase as the concentration of OH, NH, and CH chemical bonds increases.

Spectral data shows the important wavelengths of chemical bonds that represent soil characteristics and nutrients, such as OH bonds at 1430 and 1910 nm, and CHO at 1680 and 2300-2490 nm. This CHO is most likely a mineral element in the form of Fe or other mineral elements such as Bo, Mn, Cu, Zn, Mo, and Cl, which allows this NIRS to be employed as a whole owing to the synchronous vibration in a wavelength (Afriyie et al., 2022; Miranda Salazar et al., 2012). The existence of noise in the raw spectrum, which seems loose, shows the presence of noise at the moment of measurement employing Infrared spectroscopy. Then, utilizing standard normal variate (SNV) and Baseline shift correction (BSC) approaches, a spectrum correction method is required to decrease error noise in the generated NIR waves.

Spectra pre-treatment standard normal variate aims to reduce the influence of interference wave (noise). SNV has succeeded in eliminating scatter effect of the spectrum, so that the resulting spectrum is better.

Nutrients in soil are difficult to anticipate because laboratory testing is necessary, which takes time, yet the demand for nutrients must be understood instantly so that current technology can advance and plants can grow optimally. Soil nutrients must be present in appropriate amounts and in a balanced composition. Because reducing one ingredient might result in abnormal plant growth. Each nutritional element has a distinct purpose, and no one element can totally replace another.

Near infrared (NIR) technology has been widely explored and implemented as an excellent approach for quick measurement of soil and other biological quality parameters during the last several decades. Near infrared (NIR) technology has been widely researched and implemented as a quick method for analyzing soil and other biological quality parameters. NIR technology may be utilized as an alternate approach to normal chemical analysis since it is rapid, cost-effective, non-destructive, needs minimum sample preparation, and can be used immediately in the field (Sepúlveda et al., 2021). The NIR approach enables for the quantitative evaluation of many property quality parameters in a single test. This approach mainly examines the pitch and combination of basic vibrational bands in the mid-infrared range for OH bonds, NH, and CH. Based on the NIR spectrum

obtained during the model calibration procedure, the nutrient content of the soil sample was predicted (model development). The prediction model was created by regressing the NIR spectrum (variable X) with amounts of N, P, and K (variable Y) from laboratory measurements.

Calibration and validation of the spectrum Spectroscopy in the Infrared was created to forecast soil nitrogen content by correlating absorbance spectra and NIR reflectance data with soil nitrogen content data from soil laboratory studies. The total number of soil samples was 36. The spectrum produced by NIR firing on the material has 1557 spectral data points spanning the 1000-2500 nm wavelength range. Because the spectral data is still rather huge, using it as input will make it impossible for the data to attain convergence and will slow down the process; so, the next stage in data preparation is to regress the data. The principal component regression approach is used to regress spectral data (PCR). The NIR spectrum (variable X) will be regressed against levels of N, P, and K (variable Y) from laboratory measurements. The established prediction model were be validated and evaluated; the model's justification is based on the statistical parameter of the relation coefficient (r) between the prediction results and the actual measurement results, residual predictive deviation (RPD), Root mean square error (RMSE), and latent variables (LV). Prediction performance of PCR and PLSR approaches using raw untreated spectral data were presented in Fig.2.

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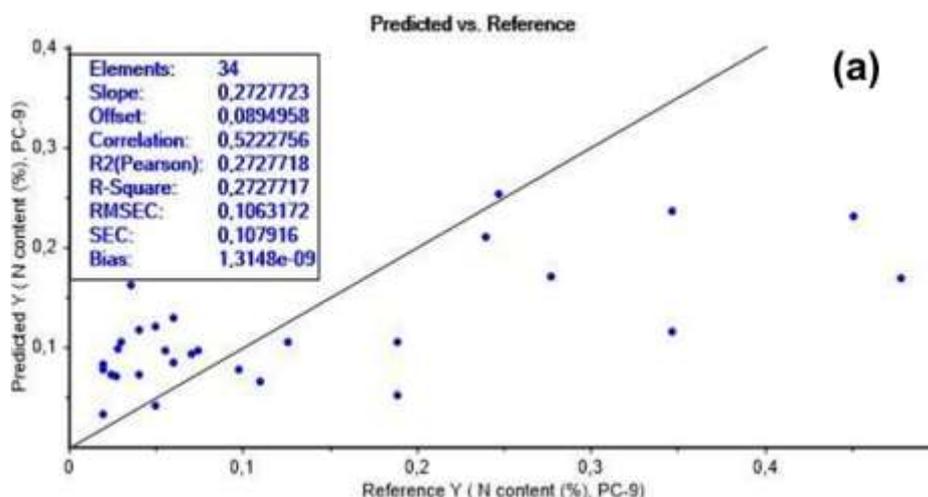


Fig. 2a—Prediction performance of PCR model based on raw spectra data



The calibration and validation outcomes of the BSC and SNV techniques are assessed using the values of R^2 , r , RMSE, and RPD. A decent calibration and validation model has an R^2 value and r that is near to 1. The RMSE is a model accuracy metric that represents the difference between the estimate and measurement results (error). The

contrast between the two low RMSEs demonstrates the model's stability. The calibration and validation models should have the same or nearly the same inaccuracy. If the RPD value is high and the latent variables are low, the predictive model is excellent.

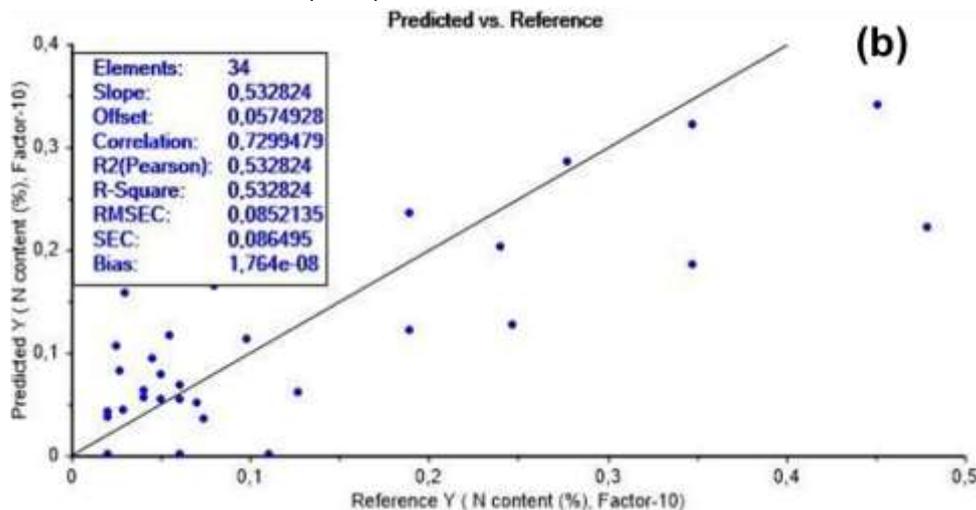


Fig. 2b–Prediction performance of PLSR model based on raw spectra data

. It showed that PLSR generate a better prediction result for N determination of soil samples. The predictions from soil testing obtained raw data with a correlation coefficient (r) of 0.73 and a value of R^2 0.53 and otherwise the value of error RMSEC is 0.08. Involved latent variables in this study, which is 10 and the RPD value of 1.5 are categorized as a coarse prediction performance and should be improved by pre-treatment like SNV and BSC approaches.

depicts the outcomes of a prediction. This is shown by an increase in the correlation coefficient (r) to 0.74. The value of the coefficient of determination (R^2) slightly increasing to 0.54 indicates a sufficient prediction, followed by the value of error (RMSEC) decreasing to 0.07 compared to the nitrogen spectrum data before correction. 0.12 is the standard deviation. The RPD index was also improved to 1.8 which is categorized as sufficient prediction performance.

The PLSR performance has increased when standard normal variate (SNV) is used. Figure 3

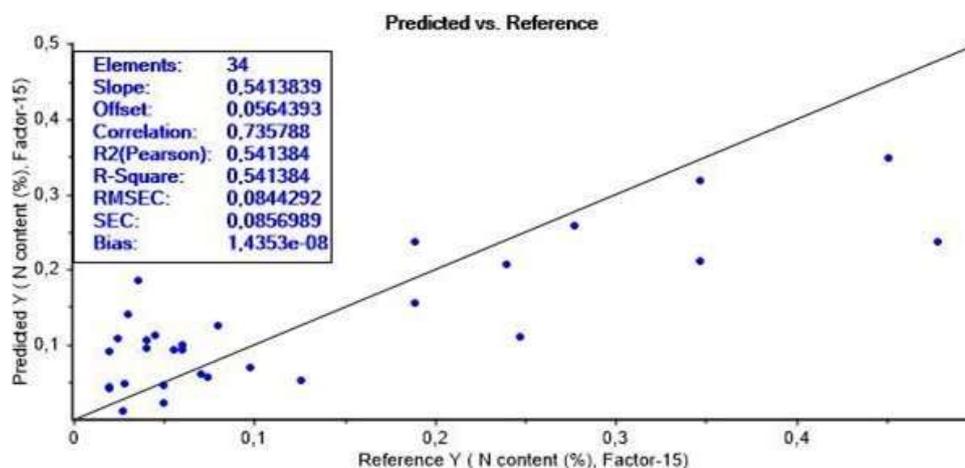
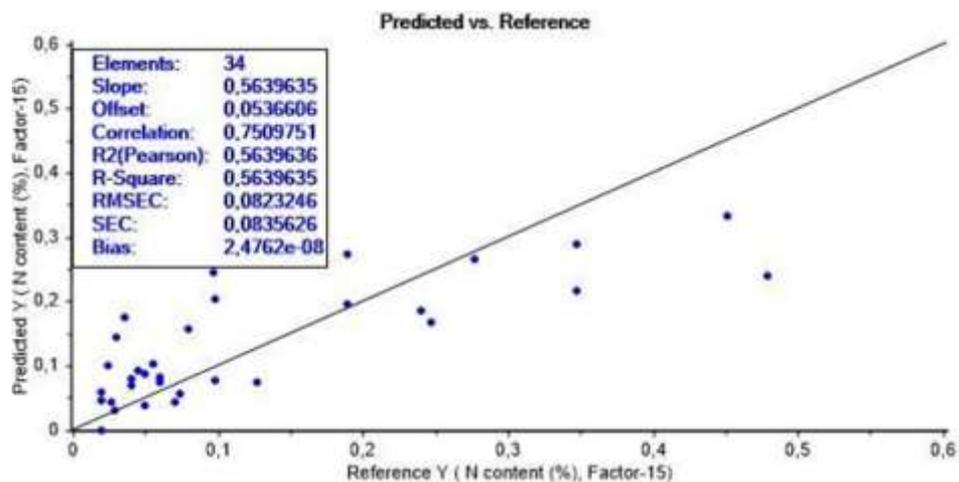


Fig. 3–Prediction performance of PLSR model based on SNV spectra data

Besides SNV, soil N prediction was also determined using another pre-treatment method namely baseline shift correction (BSC). It may increase signal by correcting the spectrum such that the sample seems to have a level ideal scatter. The calibration results after corrections were performed using the BSC spectrum correction technique is presented in Fig. 4. By upgrading the spectrum using the BSC approach, the R^2 value is

0.56 and the value of r is 0.75, indicating that the spectrum acquired above is better than the R^2 value of the prior data before being mended. The BSC approach lowered the error value (RMSEC) to 0.08 like SNV one. The RPD value is 1.92, indicating that this approach reach to a good prediction performance since the higher the RPD number, the more dependable and accurate the prediction model.



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Fig. 4—Prediction performance of PLSR model based on BSC spectra data

According to the achieved results, it is possible to say that estimating nutrient levels in soil is a positive thing and feasible to be performed using NIRS technology. Pre-treatment baseline shift correction (BSC) belonging to good model performance is best used for prediction using near infrared reflectance by method partial least square, when viewed from the acquisition of the value of r baseline shift correction (BSC) is higher, namely 0.75 and the value of R^2 baseline shift correction is 0.56. Standard normal variate (SNV) corresponding to high model performance is best employed for

prediction utilizing near infrared reflectance by technique principle component regression. The value of r standard normal variate (SNV) is greater in PCR namely 0.75, when compared to the value of r baseline shift correction (BSC), which is 0.74. Furthermore, based on loading plot analysis as shown in Fig.5, the soil NIR absorbance and reflectance spectra revealed that infrared with a wavelength of 1000-2500 nm may be utilized to forecast the soil's nitrogen levels. This is consistent with the properties of infrared wavelengths, which are sensitive to the elements C, H, O, and N.

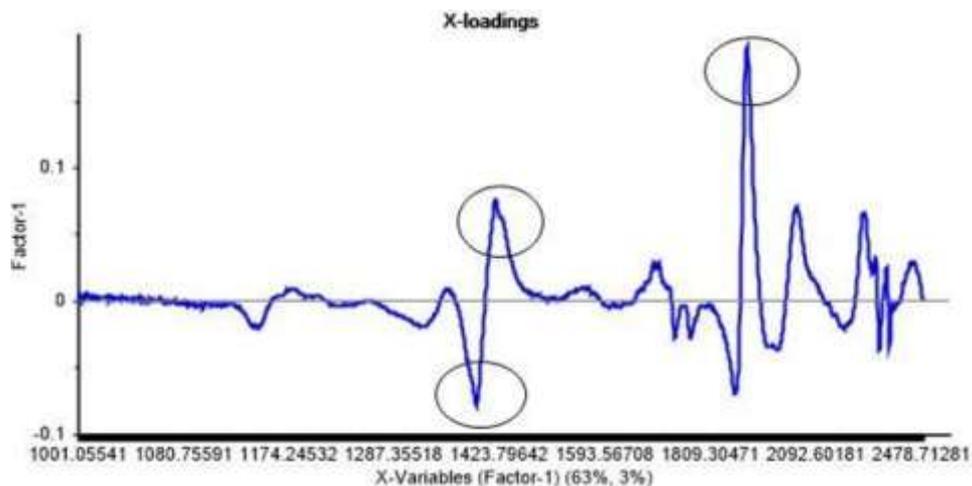


Fig. 5—Loading plot analysis based on PLSR model

Because the hydrogen atom absorbs the most powerfully NIR waves, hydrogen bonds dominate the majority of the NIR spectrum. These hydrogen bonds may take the form of CH, NH, SH, or OH bonds. Water content is shown by three absorption peaks at wavelengths of 1180 nm, 1450 nm, and 1940 nm. This absorption peak arises due to the presence of OH bonds at that wavelength. Water has a considerable impact on soil NIR spectra. Soil NIR spectra are distinguished by the absorption of the OH chemical bond, which reveals the presence of water at wavelengths between 1400 nm and 1900 nm. Spectrum of electromagnetic waves Spectroscopy in the infrared region shows how soil nitrogen may be transported by reflection and absorption. Because each organic substance's electromagnetic radiation includes various energy and photons, each organic material has different energy properties. It also depicts the peaks and troughs in the soil's NIR absorption spectra, with optimal wavelengths in the ranges of 1386-1399 nm, 1416-1436 nm, and 1898-1910 nm. The absorption in the NIR spectra of the soil at this wavelength is relatively strong, indicating the existence of C, H, O, and N bonds. Total nitrogen in the soil may be predicted by the existence of NH bonds.

4. CONCLUSIONS

Judging from prediction performances, it seems that NIRS technology can predict the soil nitrogen content in various agricultural land-use and depths. Prediction performance can be improved by establishing models by means of pre-treatments like SNV and BSC methods. The correlation coefficient was improved from 0.71

using raw model, to 0.74 and 0.76 using SNV and BSC spectral data respectively. As a consequence, the prediction error was decreased. In term of ratio prediction to deviation (RPD) index, the model is categorized as sufficient prediction performance and still can be improved by employing hybrid spectra corrections or non-linear regression approach.

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