Total Nitrogen Estimation of Paddy Soil Using Visible and Near Infrared Spectroscopy

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Abstract: The current soil nutrient estimation method is laborious, repetitive, time-consuming and costly, making it less efficient for large-scale soil fertility assessment in precision agriculture practice. This paper discussed the feasibility of visible and near-infrared (Vis-NIR) spectroscopy as an alternative method for rapid measurement of total nitrogen in the soil, which is more efficient for a huge paddy field area. For this purpose, Vis-NIR reflectance spectra (350 – 1750 nm) were acquired on 200 soil samples using spectrometers. Partial Least Squares Regression (PLSR) with full (leave-one-out) cross-validation was used to develop the calibration model between the Vis-NIR soil spectra and the total nitrogen obtained by chemical analysis in laboratory. The coefficient of determination (R²_val) and residual prediction deviation (RPD) of the developed calibration model for total nitrogen (N tot) was 0.78 and 1.86, respectively. The predicted total nitrogen map generated based on the Vis-NIR spectroscopy was comparable with the laboratory analysis’s measured map. This result indicates that the Vis-NIR infrared spectroscopy is the potential to be used for total nitrogen estimation in soil.

Keywords: visible and near infrared spectroscopy; soil nutrient; precision agriculture; total nitrogen; partial least square regression

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1. Introduction

The normal practice of uniform blanket fertiliser application, without any indication of the current level of soil nutrients, results in excessive fertiliser application in high nutrient
areas and less fertiliser application in low nutrient field zones (Thafna et al., 2017; Whetton et al., 2017). This uniform fertiliser management under spatially variable conditions can cause crop nutrient deficiencies as well as increases the in input cost due to over fertiliser application. This results in less than optimum yields and also potentially reduces environmental quality. The advancement of precision agriculture technology has led to the adoption of variable rate fertiliser application as an improved technique to replace the uniformly blanket fertiliser application. In this technique, high resolution or high-density soil nutrients information is required apart from normalised difference vegetation index (NDVI) and leaf area index (LAI) to determine the fertiliser rate that needs to be applied at a specific location (Lowenberg-DeBoer & Aghib, 1999; Maleki et al., 2008; Mouazen et al., 2009; Halcro et al., 2013; Mouazen & Kuang, 2016). In Malaysia, fertiliser recommendations by the soil service providers to the farmers are based on only one sample, over 3 to 4 ha. The conventional method of soil nutrient estimation is unable to collect the huge number of soil samples which then requires extensive, expensive and time-consuming laboratory analysis by an expert operator (Morellos et al., 2016). Therefore, an alternative method of soil nutrient assessment is needed to obtain high-density information on the soil nutrient availability for variable rate fertiliser application. This method, even if it is not as precise as the conventional method, is more cost effective, rapid and easy to use.

Proximal soil sensing has been reported as a promising technique for high-resolution soil nutrient estimation and mapping (Viscarra Rosel et al., 2010; Kuang et al., 2012). Electrical conductivity/resistivity (Corwin & Lesch, 2003), ground-penetrating radar (Lunt et al., 2005), and the γ-ray sensor (Triantafilis et al., 2013) are some of the proximal sensing techniques that have been explored. An extensive review by Kuang et al. (2012) had concluded that the most promising proximal sensing technologies for quantifying soil properties were electrochemical techniques and optical visible and near infra-red (Vis-NIR) spectroscopy. The latter technique, however, has gained the most interest because it has more advantages than others. Wijewardane et al. (2020) listed out the advantages of Vis-NIR which include its feasibility for in-situ soil sensing and the non-contact nature of interactions between Vis-NIR electromagnetic energy and soils, ease of miniaturization using optical fibres for a Vis-NIR sensing probe, and the ability to infer multiple soil properties from a single Vis-NIR scan.

In Malaysia, the use of Vis-NIR spectroscopy as an alternative technique for rapid and cost effective assessment of soil nutrients has not been reported extensively. Hence, this paper described the potential of Vis-NIR spectroscopy for the estimation of total nitrogen (N_{tot}) in paddy soil. The output from this study will be used for the development of real-time soil nutrient assessment.
2. Materials and Methods

2.1 Experimental Site and Soil Sampling

The field experiment was conducted at Rice Research and Innovation Excellence Centre (rice@MARDI) paddy field in Seberang Prai city of Penang, Malaysia (5°32′37″N 100°28′3″E). This site comprises of 10 experimental paddy field blocks with about 10 to 15 number of small paddy plots at each block. Soil samples were collected after the paddy harvesting season in October 2019. Five soil samples were collected at each randomly selected 40 paddy plots in block 1 to block 10. At each sampling location, the position coordinates were recorded using Nomad® 900 series (Trimble®, USA) integrated Global Positioning System (GPS) receiver. The collected 200 bulk soil samples were packed in air-tight plastic bags to avoid the loss of soil moisture, labelled, and immediately sent to the farmhouse near the paddy field for spectra acquisition.

2.2 Vis-NIR Soil Spectra Acquisition

Two standalone fibre type spectrometers (AvaSpec-ULS2048 and AvaSpec-NIR256, AVANTES, Netherlands) were used to obtain the Vis-NIR spectrum of the soil samples. A halogen lamp was connected to the light illumination fibre, while the detector fibres were connected to two spectrometers. The first spectrometer was a 2048-pixel CCD detector for visible and low near-infrared range (350 – 1100 nm), while the second spectrometer was a 256-pixel Indium Gallium Arsenide (InGaAs) NIR wavelength detector (900 – 1750 nm). A Vis-NIR spectrum of 350 – 1750 nm wavelengths was formed by merging both Vis and NIR spectra. Both spectrometers were connected to a laptop installed with AvaSoft 8.5 software for data logging. Figure 1 exhibits the setup for the soil spectra acquisition using the spectrometers.

![Figure 1. Experimental setup for soil spectra acquisition using the AVANTES spectrometers.](image-url)
White reference spectra were acquired using the standard reflector (Avantes WS-2 reference tile) prior to the acquisition of spectra on the soil samples, while dark reference spectra were obtained by turning off the light source. The spectra acquisition was intentionally performed on the fresh soil samples without removing the moisture through oven drying, crush and sieve so that the developed calibration model is more susceptible to the real soil condition which contains moisture and non-uniform texture as claimed by Kodaira and Shibusawa (2013). This is important towards the real-time or in-situ soil nitrogen estimation. Thus, only debris such as plant roots and stone were removed from each soil sample. Small amount of soil sample (about 20 g) was placed in a plastic Petri dish of 7.5 mm depth and 30 mm diameter. The soil surface was pressed, carefully levelled and compacted in the dish in order to get the maximum amount of reflected light. A black probe holder was used to hold the optical probe and the soil sample in the petri dish was placed underneath the probe holder. This was to ensure that the acquired spectra were not affected by the ambient light and to standardise the surface to probe distance. The petri dish was rotated at an angle 120º, and reflectance readings were acquired from each soil specimen of every rotation. At each rotation, 10 successive spectra were measured over 5 s and averaged in one spectrum for each position. The three acquired spectra at three different rotations were further averaged as a single spectrum to represent the spectrum of each soil samples. This spectra acquisition process was carried out over 200 collected soil samples. Therefore, there were 200 soil spectra that corresponded to 200 soil samples. These spectra were then used for spectral processing and model development.

After the spectra acquisition has been carried out for all the 200 samples, these samples were then sent to ESPEK Research and Advisory Services Laboratory (ERAS) for analysis of $N_{\text{tot}}$ using the combustion method.

2.3. Spectra Pre-Processing and Calibration Model Development

The spectra pre-processing and model development were performed using Unscramblers software (Version X10.2, Camo A/S, Oslo, Norway). All collected 200 soil reflectance spectra were converted to absorbance by applying the Beer-Lambert's law (Williams & Norris, 2001) as in Equation 1;

$$A = \log_{10}(R_w - R_d) - \log_{10}(R - R_{\text{dark}}) \quad (1)$$

$R_w$ is white reflectance spectra using the standard reflector, $R_d$ is dark reflectance spectra when the light source was turned off, whereas $R$ denotes the reflectance spectra of the soil samples. In order to obtain all data at approximately the same scale, the maximum normalization technique was applied to the average absorbance spectrum. The second derivative Savitzky and Golay pre-treatment method was further applied to the absorbance spectra to enhance weak signal and reduce the diffusive reflectance noise.
The $N_{\text{tot}}$ calibration model was developed using the partial least-square regression (PLSR) technique validated using full cross-validation to establish the correlation between the values of $N_{\text{tot}}$ from the laboratory-chemical analysis (reference values) and the pre-processed Vis-NIR soil absorption spectra of each respective locations. The coefficient of determination ($R^2_{\text{val}}$) and residual prediction deviation (RPD) produced from the PLSR analysis of the developed model was used to evaluate the accuracy of the model. RPD is a ratio of the standard deviation (SD) of the reference dataset to the full cross-validation root mean square error (RMSE$_{\text{val}}$), as in Equation (1) (Chang et al., 2001; Cozzolino et al., 2005; Mouazen et al., 2006) was calculated from the validation dataset using Equation 2 (Brereton, 2003)

$$\text{RPD} = \frac{\text{SD}(y_{m})}{\text{RMSE}_{\text{val}}}$$  \hspace{1cm} (2)

2.4. Validation and Map Comparison

The developed calibration model was validated on 72 Vis-NIR soil spectra that were acquired at plot 12 in block 5 in the following season (February 2020). Seventy-two soil samples were also collected at the same location and sent to the same laboratory for analysis of $N_{\text{tot}}$. The model was applied to the collected validation spectra to obtain the predicted $N_{\text{tot}}$.

Two maps of plot 12 from block 5 were then generated using the ARCVIEW GIS 3.1 software. The first map was the measured map which was generated based on the amount of $N_{\text{tot}}$ obtained from the laboratory analysis while the second map was a prediction map generated based on $N_{\text{tot}}$ prediction values computed by Vis-NIR calibration model. Inverse distance weighing (IDW) method was applied to interpolate both maps.

3. Results

The $N_{\text{tot}}$ statistics of the calibration and validation (prediction) sets for a total of 200 soil sample are listed in Table 1 while the PLSR analysis result of the calibration model is shown in Table 2. The acquired raw and pre-treated absorbance Vis-NIR spectra are depicted in Figure 2. Both ends of the Vis-NIR absorbance spectra were deleted as these spectra regions were unstable and high in noise. The calibration model was then developed on the final 200 spectra with wavelength range from 480 to 1600 nm at 5 nm interval. Moreover, a total of 20 samples outliers (10% of the dataset) were detected and removed from the model dataset. The scatter plot of the model for $N_{\text{tot}}$ is depicted in Figure 3. The primary regression equation for $N_{\text{tot}}$ is also shown. The measured and predicted digital map of $N_{\text{tot}}$ for validation plot 12 in block 5 is illustrated in Figure 4.
Table 1. Statistical results of soil chemical analysis on N_{tot} in calibration dataset from 200 soil samples.

<table>
<thead>
<tr>
<th>Statistic</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Min</td>
<td>0.02</td>
</tr>
<tr>
<td>Max</td>
<td>0.30</td>
</tr>
<tr>
<td>Mean</td>
<td>0.14</td>
</tr>
<tr>
<td>Range</td>
<td>0.28</td>
</tr>
<tr>
<td>Std Dev</td>
<td>0.04</td>
</tr>
</tbody>
</table>

Figure 2. The merged of 200 Vis-NIR spectra for developing the calibration model. (a) original absorbance spectra and (b) pre-treated spectra.
Table 2. PLSR result for calibration model of $N_{\text{tot}}$.

<table>
<thead>
<tr>
<th></th>
<th>$R$</th>
<th>$R^2$</th>
<th>RMSE</th>
</tr>
</thead>
<tbody>
<tr>
<td>calibration</td>
<td>0.89</td>
<td>0.80</td>
<td>0.014</td>
</tr>
<tr>
<td>validation</td>
<td>0.88</td>
<td>0.78</td>
<td>0.021</td>
</tr>
</tbody>
</table>

Figure 3. Scatter plot of measured values versus Vis–NIR predicted values using PLSR coupled with full cross-validation datasets for $N_{\text{tot}}$.

Figure 4. Comparison of (a) measured and (b) predicted map of $N_{\text{tot}}$ for validation plot 12 in block 5.

4. Discussion

The accuracy of the calibration was evaluated based on the ($R^2_{\text{val}}$) in cross-validation, and the RPD. $R^2_{\text{val}}$ indicates that the percentage of the variance in the Y variable is accounted for by the X variable. Williams (2003) suggested that an $R^2_{\text{val}}$ of between 0.50 and 0.65 means that more than 50% of the variation in Y is accounted for by variable X, so that high and low levels can be discriminated. An $R^2_{\text{val}}$ shows estimated quantitative predictions between 0.66
and 0.81, while an $R^2_{val}$ shows a strong prediction between 0.82 and 0.90. The calibration model is considered to be outstanding with an $R^2_{val}$ above 0.91 (William, 2003). Based on this classification, the $R^2_{val}$ of 0.78 obtained in this study indicated that the developed model can be used for quantitative prediction of $N_{tot}$.

According to Chang et al. (2001), the RPD value is considered excellent when it is above 2.0, nearly good between 1.4 and 2.0 and unreliable the value falls below 1.4. It was found from this classification that the performance of the developed model for predicting $N_{tot}$ is good (RPD = 1.86). The comparative maps between the measured and predicted maps shown in Figure 3 indicated that a partial similarity distribution of $N_{tot}$ in most parts of plot 12 in block 5. The measurement ranges obtained using the two techniques were very similar. This indicated that the spatial distribution of $N_{tot}$ based on the Vis-NIR spectroscopy along with their location coordinates is reliable and can be used to generate a digital soil nitrogen map so that the nitrogen distribution in the soil can be seen visually. The digital map can then be used to assist farmers or agronomist in making decision for site-specific variable-rate fertiliser application. In addition, the estimated nitrogen values combined with the paddy plant nitrogen content can also be used as an input for the on-the-go variable rate fertiliser applicator.

The reliability and robustness of the calibration models should be improved, which will then increase the quality of the maps generated in the future. One of the suggestions in further studies is to provide more soil samples in other regions of Malaysia from different types of cultivation fields in order to have greater diversity in soil properties. It is also important to evaluate the independent validation set model to examine whether it would be robust or restricted to the conditions under which the calibration samples were collected. It is also appropriate to take into account a wider spectral range, potentially up to 2500 nm, as perhaps more substantial absorption characteristics are available for $N_{tot}$ between 1700 and 2500 nm. However, due to the higher pricing required for higher wavelength spectrometers, the efficiency of using a wider range of NIR must be weighed as the higher range of spectra wavelength is costly. Although the predicted Vis-NIR map did not fit the corresponding observed map perfectly, the identical distribution pattern that existed between the two maps is sufficient to declare that Vis-NIR spectroscopy is a promising technique for estimating and mapping total nitrogen in paddy soil.

5. Conclusions

A spectroscopic calibration model for $N_{tot}$ was developed based on Vis-NIR soil reflectance spectra acquired by commercial spectrometers on soil samples collected from 10 blocks of paddy plots. The performance of the developed model was found to be good for the quantitative prediction of $N_{tot}$. The comparable maps generated based on the spectroscopic technique's prediction indicated that this technique and their location coordinates recorded by GPS can be used for estimation and digital mapping of $N_{tot}$ distribution in paddy soil.

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Conflicts of Interest: The authors declare no conflict of interest.

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