Environmental assessment of soil quality indices using near infrared reflectance spectroscopy

D Devianti1*, Sufardi2, S Syafriandi1, A A Munawar1

1Department of Agricultural Engineering, PUSMEPTAN Universitas Syiah Kuala, Jalan Tgk. Hasan Krueng Kalee 3, Banda Aceh 23111, Indonesia
2Department of Soil Science, Universitas Syiah Kuala, Jalan Tgk. Hasan Krueng Kalee 3, Banda Aceh 23111, Indonesia

*Email: devianti@unsyiah.ac.id

Abstract. The main purpose of this preset study is to assess soil quality indices in form of potassium (K) and phosphorus (P) contents using a non-invasive and environmental friendly approach namely near infrared reflectance spectroscopy. Soil samples were obtained from Aceh Besar district in rice field land-use. Near infrared spectral data of soil samples were acquired and recorded as absorbance in wavelength range from 1000 to 2500 nm. On the other hand, actual P and K were measured using standard laboratory procedures by means of Kjeldahl methods. Spectral data were corrected and pre-treated using mean centering approach and applied to all dataset. Prediction models were developed using principal component regression and validated using leverage cross validation. The results showed that both soil quality indices can be predicted with maximum correlation coefficient (r) of 0.98 and ratio prediction to deviation (RPD) index of 3.47 for P, and r of 0.91, RPD of 2.68 for K respectively. It may conclude that environmental assessment, particularly for soil quality determination can be conducted rapidly and non-invasively using near infrared spectroscopy approach.

1. Introduction
Soil is a natural object found on the surface consisting of mineral and organic materials and has physical, chemical, biological properties, and has the ability to support human life and other living things. the result of mineral materials as from weathering rocks, and organic materials as weathering of plant and animal remains, which is a place for the growth of plants with certain characteristics, which occur due to the combined influence of climatic factors, materials, and formation time [1].

Soil has various functions, particularly in agriculture it is used as a medium for plant cultivation. Land resources in Indonesia that are used as production land for cultivation are divided into 3 categories, namely cultivation of food crops, plantation crops, and horticultural crops, like fruit, vegetable, ornamental, medicinal and aromatic plants [2–4]. The properties of soil fertility, namely physical fertility, chemical fertility, and soil fertility affect plant growth. Physical fertility prioritizes the physical condition of the soil which provides more air and soil facilities, while the fertility properties concern the availability of nutrients for plant growth [5–7].

Plant growth is directly proportional to soil fertility. It is the ability of the soil to provide nutrients needed by plants to support their growth and reproduction. Depletion of soil fertility is partly due to loss of nutrients from the soil, and can occur through crop harvesting (nutrient harvesting), runoff, and
leaching. Nutrient loss due to harvesting depends on the amount produced and the method of harvesting. Provision of nutrients that have been lost can be done by adding fertilizer which is the key to soil fertility. Phosphorus (P) is a macronutrient that plants need in large amounts and is essential for plant growth. Phosphorus is often referred to as the key to life because it is directly involved in almost all life processes. In the plant body, P plays an important role in several cell division activities and the formation of fat and albumin, the formation of flowers, fruits, and seeds, plant maturity against the effects of nitrogen, stimulates root development, improves crop yield quality and resistance to pests and diseases [8]. Phosphorus plays a role in stimulating root growth. This is evidenced from the results of experiments on soils lacking phosphorus, when added, it turns out that the root portion is greater than the top of the plant, especially the leaves [9,10].

On the other hand, Potassium (K) is a macro nutrient that plants need in large quantities to grow and produce. Nutrient K is not a constituent element of plant tissue, but plays a role in the formation of starch, functions as an enzyme activator of about 80 types of enzymes whose activation requires K elements, helps the absorption of water and other nutrients from the soil by plants and helps transport assimilated products from the leaves to the soil. plant tissue [11,12].

The method that can be used as an alternative to quickly estimate soil nutrient content is using Near-infrared reflectance spectroscopy (NIRS). This technique has become one of the most promising non-destructive methods that can be used in various fields, including agriculture [13–15]. NIRS has several advantages over traditional (conventional) chemical analysis because it is carried out non-destructively, can analyze samples to a depth of 2-5 millimeters, can detect various components with one spectral data. Thus, the main purpose of this present study is to assess soil quality indices in form of potassium (K) and phosphorus (P) contents using a non-invasive and environmental friendly approach namely near infrared reflectance spectroscopy.

2. Materials and methods

2.1. Soil samples
The material used in this study is soil from paddy field in several areas of Aceh Besar District. Soil samples were taken from each site with a depth of 0-30 cm in each different rice field plot [16].

2.2. Near infrared spectra acquisition
Near infrared spectral data of soil samples were acquired and recorded as absorbance in wavelength range from 1000 to 2500 nm using a portable sensing device PSD NIRS i16 as shown in Figure 1.

![Figure 1. PSD NIRS i16 for spectral data acquisition of soil samples](image-url)
2.3. Soil quality prediction
Soil quality indices in from of potassium (K) and phosphorus (P) contents were predicted by establishing models used to determine both quality indices [8]. These models were developed using principal component regression and validated using leverage cross validation.

2.4. Prediction models evaluation
In order to justify the accuracy and robustness of the models, several statistical parameters were introduced namely correlation coefficient (r), root mean square error (RMSE) in calibration and cross validation, ratio prediction to deviation (RPD) as follows:

\[
\tau_{xy} = \frac{\sum_{i=1}^{n} (x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_{i=1}^{n} (x_i - \bar{x})^2 \sum_{i=1}^{n} (y_i - \bar{y})^2}}
\]

\[
\tau_{xy} = \frac{1}{n-1} \sum_{i=1}^{n} \left( \frac{x_i - \bar{x}}{s_x} \right) \left( \frac{y_i - \bar{y}}{s_y} \right)
\]

\[
\text{RMSD} = \sqrt{\frac{\sum_{t=1}^{T} (x_{1,t} - x_{2,t})^2}{T}}
\]

It is obvious that good prediction models should have high correlation coefficient and ratio prediction to deviation index. In contrast, should have lower root mean square error (RMSE) in calibration and cross validation [17–20].

2.5. Optimum wavelengths for soil quality indices
The most relevant and optimum wavelengths for soil quality indices prediction were determined by looking the peak and valley in regression coefficient plot or loading plot.

3. Results and discussion
3.1. Spectra features of soil samples
The texture features which comprise the contrast, correlation, energy, homogeneity, and entropy of the nutmeg quality are shown in figure 2.
Samples subjected to near infrared radiation with a wavenumber of 1000-2500 nm will receive energy that triggers vibrations and strains in the molecular bond groups of O-H, N-H, and C-H atoms which are the main components forming organic compounds and due to the interaction of molecular bonds can indicate soil nutrient content. Some of the energy will be absorbed and some will be reflected. The energy emitted into organic materials, about 4% will be reflected back to the outer surface (regular reflection) and about 96% will enter the material and then undergo absorption, reflection, scattering and transmitting light. Score plot of the PCA analysis derived from three principal components of various soil land-use are presented in figure 3 and figure 4 respectively.

![Figure 3. Principal component analysis plot of soil spectral data.](image1)

![Figure 4. Principal component analysis score plot of different various land-use.](image2)

For plants, fertilizer is like food for humans. By plants, fertilizers are used to grow, live, and thrive. If in human food there is a nutritional term, then in fertilizer it is known as a substance or nutrient element. Nutrient content in plants varies, depending on the type of nutrient, type of plant, soil fertility or species, and different plant cultivation. In general, it can be said that the benefits of fertilizers are to
provide nutrients that are lacking or even not available in the soil to support plant growth. The content of elements in fertilizers will also produce different fertilizer colors. There are fertilizers that are black because they contain a lot of humus or peat, there are fertilizers that are gray in color, such as TSP fertilizer, because they are taken from phosphate rock of that color, and there are also fertilizers that are pure white in color, such as urea as a result of chemical processes of elements. nitrogen. As a material that is added to the soil or plant canopy with the aim of complementing the availability of nutrients, the required fertilizer consists of macro and micro fertilizers.

Soil quality assessment by means of NIRS approach can be performed by establishing prediction models used to determine several quality parameters simultaneously. Spectral data were also subjected onto regression method namely principal component regression consisting X variable as spectra data and Y variable of P and K values. At first, raw spectra data were used to develop the PLS models for P and K prediction as shown in Figure 5 and Figure 6 respectively.

![Figure 5](image1.png)

**Figure 5.** Prediction performance of PLS-raw spectrum for P soil determination.

![Figure 6](image2.png)

**Figure 6.** Prediction performance of PLS-raw spectrum for K soil determination.

Macro nutrients are needed for plant growth in large quantities in order to obtain high yields. The macro-nutrients are N, P, K, C, H, O, Ca, Mg and S. Micro-nutrients function as forming chlorophyll or leaf green and photosynthesis rate, enzyme-forming material, improving root function. Needed in small quantities. The micro nutrients are Cu, Zn, Bo, Cl, Fe and Mn. The chemical nutrients needed by lowland rice plants are generally Urea, SP36, KCl, and NPK compound fertilizers. Inorganic chemical fertilizers
are used to increase the lack of nutrients needed by plants to achieve a certain level of yield, if the nutrients naturally available from the soil are insufficient. Prediction performances were improved significantly when the models are constructed using corrected spectral data namely peak normalization (PN) as shown in Figure 7 and Figure 8.

Phosphate exists in three forms, namely H$_2$PO$_4^-$, HPO$_4^{2-}$, and PO$_4^{3-}$. Phosphate is generally absorbed by plants in the form of primary orthophosphate ion H$_2$PO$_4^-$ or secondary orthophosphate HPO$_4^{2-}$ while PO$_4^{3-}$ is more difficult to be absorbed by plants. The most dominant form of the three phosphates in the soil depends on the soil pH. Plants that have a low pH absorb more primary orthophosphate ions, and at a higher pH, plants absorb more secondary orthophosphate ions. Sources of phosphate in the soil as mineral phosphate are limestone phosphate, plant debris and other organic matter. The conversion of organic phosphorus to inorganic phosphorus is carried out by microorganisms. In addition, the absorption of phosphorus is also carried out by clay and silicates.

Inorganic and organic phosphates are found in the soil. The inorganic forms are compounds of Ca, Fe, Al, and F. Organic phosphorus contains compounds derived from plants and microorganisms and is composed of nucleic acids, phospholipids, and phytin. The inorganic form of soil phosphorus is less and less soluble. Even though there is CO$_2$ in the soil, neutralizing phosphate is still difficult, so that the
available P in the soil is relatively low. Phosphorus available in the soil can be interpreted as P soil that can be extracted or soluble in water and citric acid. P-organic with the decomposition process will become inorganic form.

The availability of potassium in the soil is strongly influenced by several factors, namely the type of soil colloid, temperature, soil pH and weathering. The relationship between soil pH and the amount of K- is opposite. This means that potassium fixation occurs at high soil pH, so that at that soil pH potassium can be exchanged to be low. This can be caused by increasing soil pH or adding calcium causing the adsorption complex to saturate with calcium. Thus, more potassium will be bound because calcium will bind to Cl, if fertilizer is given KCl, so K-dd will be reduced in the soil. On the other hand, at low pH, K-dd is quite high because potassium fixation is relatively low.

4. Conclusions
Presented study aimed to assess soil quality indices in form of potassium (K) and phosphorus (P) contents using a non-invasive and environmental friendly approach namely near infrared reflectance spectroscopy. Near infrared spectral data of soil samples were acquired and recorded as absorbance in wavelength range from 1000 to 2500 nm. Spectral data were corrected and pre-treated using mean centering approach and applied to all dataset. Prediction models were developed using principal component regression and validated using leverage cross validation. The results showed that both soil quality indices can be predicted with maximum correlation coefficient (r) of 0.98 and ratio prediction to deviation (RPD) index of 3.47 for P, and r of 0.91, RPD of 2.68 for K respectively. It may conclude that environmental assessment, particularly for soil quality determination can be conducted rapidly and non-invasively using near infrared spectroscopy approach.

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