Impact of Near Infrared Spectra Corrections to The Prediction Performance of Soil Macro Nutrients

Yuswar Yunus, Devianti, Purwana Satriyo, Agus Arip Munawar

Abstract: This present study aimed to apply and compare three different spectra data correction methods to the overall prediction performance of near infrared calibration models used to determine soil macro nutrients. Those three spectra correction methods are: de-trending (DT), mean centering (MC) and Savitzky-Golay smoothing (SGS). Near infrared spectra data of soil samples were measured and recorded in wavelength range from 1000 to 2500 nm. Soil samples were collected in 5 and 20 cm depth respectively in rice field area in Aceh Besar district, Aceh Province. Moreover, calibration models were built to predict soil macro nutrients in form of Nitrogen (N) and Calcium (Ca). Partial least square (PLS) regression was employed to construct those models. The results showed that spectra corrections provided a better prediction performance compared to un-corrected spectra (raw). The maximum determination coefficient achieved were 0.94 for N prediction, and 0.97 for Ca prediction respectively. Thus, it may conclude that spectra corrections definitely affected to the overall prediction performances of soil macro nutrient contents.

Index Terms: Spectra, NIRS, Soil, Agriculture, Macro nutrient, prediction, technology.

---

1. INTRODUCTION

In many agricultural practices, soil is an important media for plants to grow. They need a complete package of macro and micro nutrients for their sustainable growth. If this requirement is met, they can produce high quality agricultural products. Fulfillment of plant nutrient needs is an absolute thing to do, because the availability of nutrients in nature is very limited, and decreases because it has been absorbed by plants [1], [2]. The nitrogen is a macro nutrient, and absolutely needed by plants. It stimulates the overall vegetative growth of plants, especially the growth of roots, stems and leaves. Nitrogen also play an important role in the formation of leaf green substances (chlorophyll) which is very important to carry out the process of photosynthesis [3]. In addition, nitrogen also involved in the formation of protein, fat and various other organic compounds. On the other hand, calcium Serves to stimulate the formation of root hairs, harden plant stems and stimulate seed formation. Calcium in stems and leaves is useful for neutralizing compounds or conditions that are unfavorable to the soil. Both calcium and nitrogen must be provided in an optimum amount, because lack or excessive amount of macro nutrient contents can also affect to the plant growth [4].

Symptoms of plants that lack of nitrogen content: plant growth is slow, thin and stunted plants, yellowish green leaves, short, small and upright, old leaves are light green, then turn yellow, wither and the fruit will be stunted. On the other hand, if soil have an excessive amount of nitrogen, it will produce young and weak plants, grain production is reduced, slows in ripening of fruit and seeds [5]. Furthermore, several symptoms caused due to lack of calcium content in soil are: the edges of young leaves will turn yellow due to chlorosis, which then radiates to the leaf bone. Young buds will die because the roots are less than perfect. If a leaf grows, the color will change and some of the tissue in the leaf will die [6]. Based on this point of view, soil macro nutrients must be monitored and controlled precisely. They need to be determined rapidly in a real-time sequence, in order to maintain soil quality in a fertile condition [7]. Normally, soil quality either as macro or micro nutrient contents, were determined and measured using several standard laboratory procedures which are time consuming, laborious, involved chemical materials and thus can cause environmental pollutions [8], [9]. The development of non-destructive and rapid method in a real time situation in agricultural field is more attractive and gaining more attentions. These methods can be used to predict and determine several quality attributes in a short time and without involving chemical materials [10]. One of those methods is the application of near infrared reflectance spectroscopy or NIRS. This method can predict several parameters simultaneously with one spectra acquisition [11]. The NIRS was widely applied in many fields including in agriculture like fruit and horticulture products [12], [13], feed and animal products [14], [15], crops and agricultural products [16]–[18], and also for soil quality determination [8], [19]. A major consideration in NIRS application is obtained spectra data used to construct calibration models. Technically, raw spectra data can directly be used to develop those models for prediction purposes. However, based on previous studies, the prediction performances, accuracy and robustness are sometimes below expectations. Therefore, spectra data needs to be corrected and enhanced in order to improve overall prediction performances. There widely spectra correction methods used to enhance near infrared spectra datasets like smoothing, normalization, shifting, centering and scaling, and spectra transformations [20]. Numerous studies reported that spectra corrections and pre-processing before calibration models can improve prediction accuracy and robustness of several quality attributes of agricultural products [21], [22]. Thus, the main purpose of this present study is to apply and compare the impact of several spectra correction algorithms to the prediction of nitrogen and calcium contents of agricultural soil.

- *All authors are currently working at the Department of Agricultural Engineering, and PUSMEKTAN Syiah Kuala University, Jl. T Hasan Krueng Kalee No.3, Darussalam Banda Aceh 23111 – Indonesia.*
- *Corresponding author: yuswaryunus@unsyiah.ac.id*

2 MATERIALS AND METHODS

2.1 Soil samples
Soil samples were obtained from rice filed in several area of Aceh Besar district, Aceh Province, Indonesia. Soil samples were collected as top soil at 5 cm and 20 cm depth.

2.2 Near infrared spectra data
The near infrared spectra data of collected soil samples were acquired and recorded using a portable sensing device (PSD) infrared spectroscopy NIRS i16 in wavelength range from 1000 to 2500 nm with an increment of 0.2 nm and optical gain 4x. Spectra data were recorded as absorbance and saved in local computer for further analysis [23].

2.3 Soil macro nutrients measurement
Soil nitrogen content was measured and determined using the Kjeldahl method with digestion by H_2SO_4 and expressed in percentage of their weight to the total weight of dry soil sample. Furthermore, soil macro nutrient as calcium content wss measured and determined using absorption flame with an acid digestion method and coupled inductive plasma [24].

2.4 Spectra correction
To study the impact of spectra correction to the prediction performance, spectra data were corrected and enhanced using three different spectra correction methods and algorithms namely: de-trending (DT), mean centering (MC) and Savitzky-Golay smoothing (SGS) [6], [25].

2.5 Prediction models
The core step in near infrared spectroscopy application is to construct calibration models used to predict and determine several quality parameters of studied object. In this study, prediction models were developed to determine nitrogen and calcium contents of soil samples using raw and corrected spectra data. Prediction models were developed using partial least square (PLS) regression approach followed with leverage cross validation [6], [26]. Prediction models performance were evaluated and justified based on their accuracy and robustness in determining soil macro nutrient contents by means of these following statistical parameters: correlation coefficient (r) or coefficient of determination (R^2) between the prediction results and actual measurement and the ratio prediction to deviation (RPD) [27], [28].

3 RESULTS AND DISCUSSION
The spectra feature of soil samples in near infrared region consisted of absorption bands in certain wavelengths corresponds to specific soil quality attributes such as macro and micro nutrients, moisture content and mineals. The absorbance spectrum of soil samples in 5 cm and 20 cm depth is presented in Fig.1.

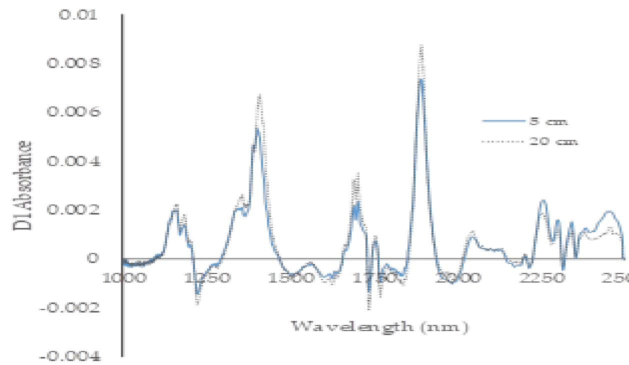

Fig. 1. Spectra feature of soil samples at 5 cm and 20 cm depth

The portion of absorbance spectrum in NIR region reflected the amount of light absorbed by the chemical constituent of soil samples where in this case soil macro and micro nutrients. The moisture contents of soil samples normally absorbed more light in wavelength 1460 and 1920 nm [7], [26]. On the other hand, soil macro nutrients generally absorbed more light in wavelength 1827 – 2100 nm. Descriptive statistics of actual soil macro nutrients is presented in Table 1. First of all, prediction models were developed using raw original un-corrected spectra data. They were used to predict both nitrogen and calcium contents simultaneously using the partial least square (PLS) regression approach. The prediction performance of N and Ca predictions was presented in Fig. 2.

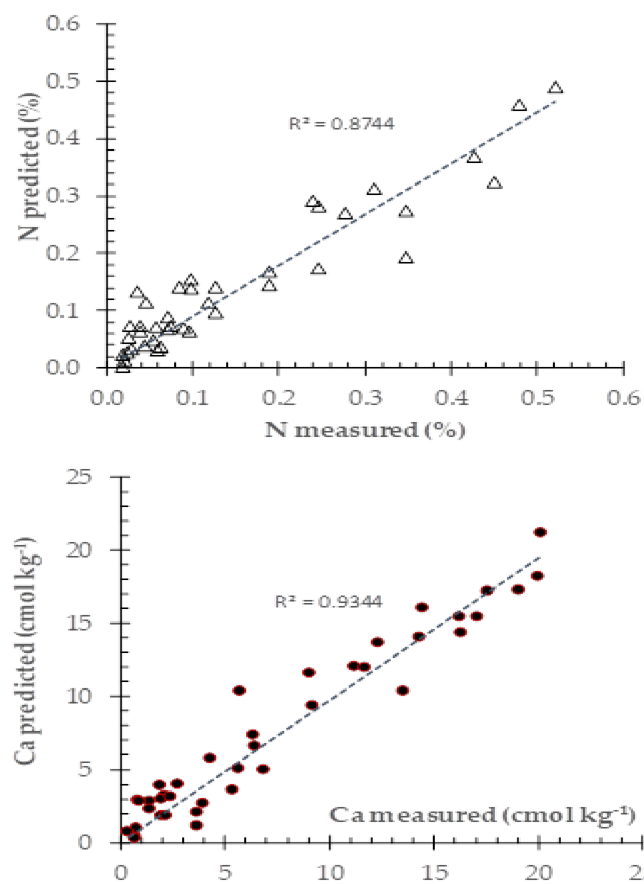

Fig. 2. Prediction performance of N and Ca contents using raw un-corrected spectra data.

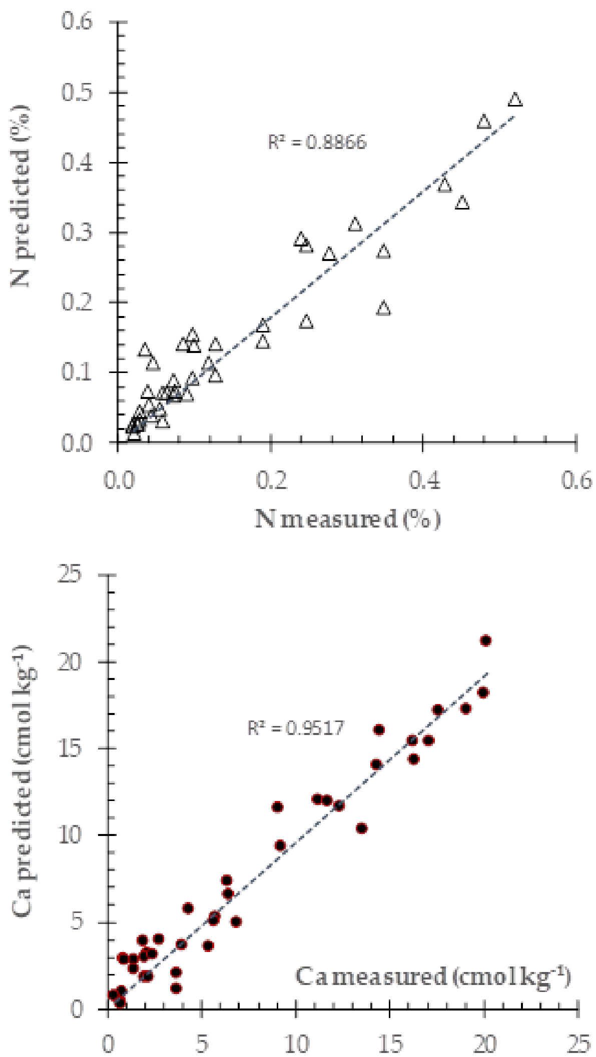

Fig. 3. Prediction performance of N and Ca contents using Savitzky-Golay

As shown in that figure, the prediction performance using raw spectra data provide quire robust and accurate prediction results. The coefficient of determination (R^2) for N prediction reach 0.8744 while for Ca prediction the R^2 coefficient achieve 0.9344. It shows that NIRS has the ability to determine those both soil macro nutrients rapidly and simultaneously. In order to achieve more robust and accurate prediction results, calibration models were also established using corrected spectra data. Smoothing was chosen as the first method to correct spectra data since this method is simply and correct some noises due to minor light scattering and amplifications. The prediction performance using smoothing spectra data proven to be more accurate and robust in predicting N and Ca as presented in Fig.3.

TABLE 1

DESCRIPTIVE DATA OF ACTUAL SOIL MACRO NUTRIENTS

Descriptive statistics	N	Ca
Mean	0.15	7.45
Max	0.52	20.18
Min	0.02	0.39
Range	0.50	19.79
Std. Deviation	0.14	6.41
Skewness	1.25	0.68
Kurtosis	0.47	-0.95
Median	0.09	5.55

The prediction performance clearly was improved when the models are constructed using corrected spectral data where in this case by means of smoothing algorithm. The R^2 coefficient was increased to 0.8866 for N, and 0.9517 for Ca prediction. Moreover, the models were also established using another corrected spectra data using mean centering (MC). The mean centering algorithm seek to remove amplifications and additives effect of light scattering by centered spectra data to its ideal spectrum which is normally mean spectra data. Acquired spectra data from studied samples sometimes may contain irrelevant background information and noises which can affect and interfere soil fertility properties such as soil macro nutrients or other contents. Prediction performance of N and Ca of soil samples using mean centering (MC) spectra data is presented in Fig. 4.

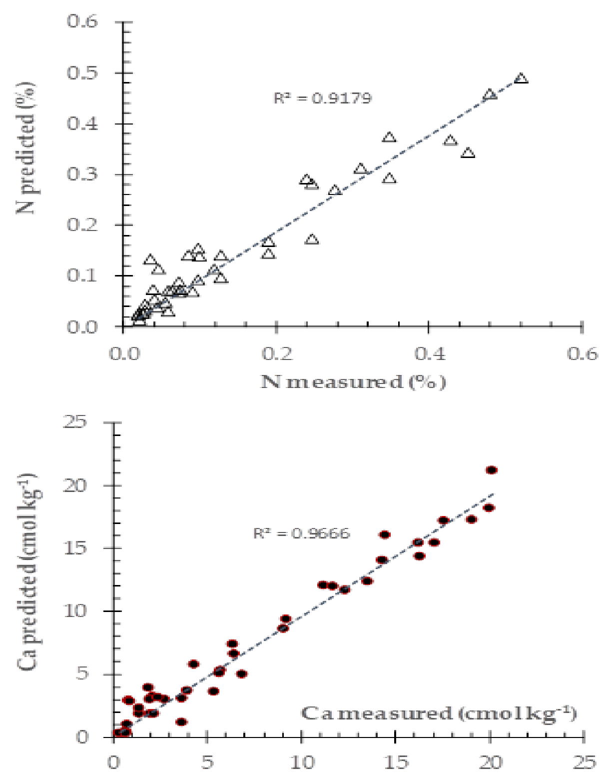

Fig. 4. Prediction performance of N and Ca contents using Mean centering (MC) spectra data.

Interfering spectra data such as light scattering and other random noises due to light scattering, overheated sensors, other NIRS instrument parts and physical sample changes. Prediction performance of soil macro nutrients were improved when the models is established using mean centering spectra data. It generated more accurate and robust prediction performance with R^2 coefficient 0.9179 for N content prediction, while for Ca prediction, the R^2 coefficient was 0.9666 respectively. Furthermore, calibration models was also developed using de-trending spectra data. It attempted to remove several noises due to light scattering, curvature effect and other temperature effects. The prediction performance of N and Ca contents using de-trending spectra data is presented in Fig. 5.

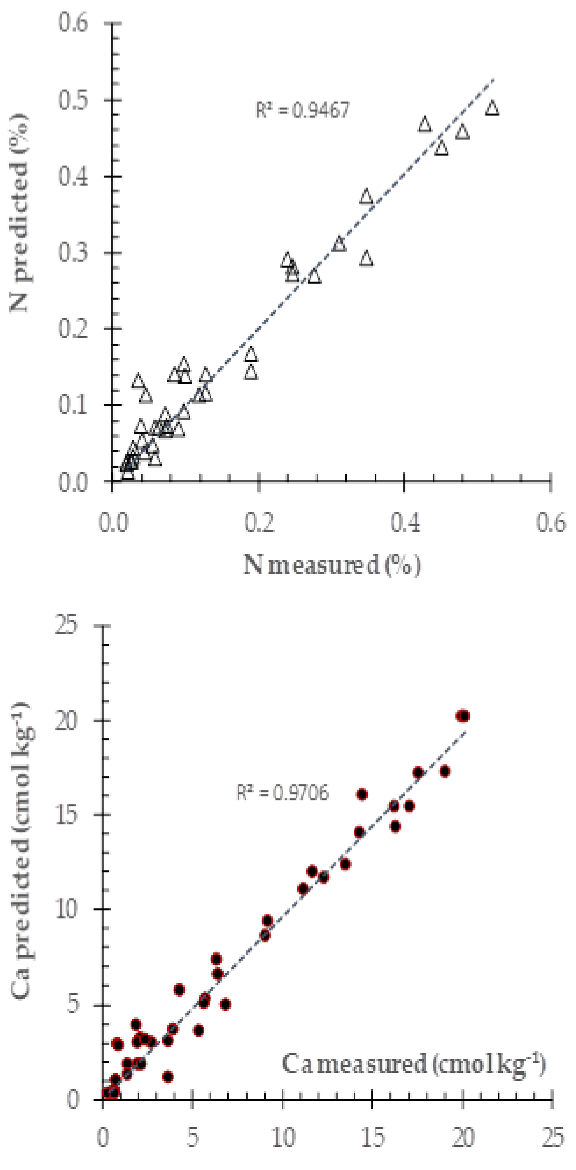

Fig. 5. Prediction performance of N and Ca contents using De-trending (DT) spectra data.

Based on obtained results, the de-trending spectra correction generated most robust and accurate prediction results both for N and Ca contents of soil samples. The maximum determination coefficient for nitrogen prediction is 0.9467, and for calcium prediction is 0.9706. It showed that proper spectra algorithms can affect overall prediction performance of near infrared spectroscopic calibration models.

4 CONCLUSION

The impact of different spectra correction algorithms to the prediction performance is investigated. The models are established using raw and corrected spectra data namely: smoothing, mean centering and de-trending to determine soil macro nutrients in form of N and Ca content using partial least square regression approach. Based on obtained results, it may conclude that NIR spectroscopy is feasible to be used for soil quality parameters prediction. Moreover, spectra corrections are highly affected to the prediction performance.

5 ACKNOWLEDGMENT

Authors wish to thank and sincere acknowledge to the division of research and community services (LPPM) Syiah Kuala University for research funding and support through Penelitian Profesor (PP) research scheme 2020.

REFERENCES

[1] T. Shi, J. Wang, Y. Chen, and G. Wu, “Improving the prediction of arsenic contents in agricultural soils by combining the reflectance spectroscopy of soils and rice plants,” Int. J. Appl. Earth Obs. Geoinf., vol. 52, pp. 95–103, 2016, doi: 10.1016/j.jag.2016.06.002.

[2] C. Tao, Y. Wang, W. Cui, B. Zou, Z. Zou, and Y. Tu, “A transferable spectroscopic diagnosis model for predicting arsenic contamination in soil,” Sci. Total Environ., vol. 669, pp. 964–972, 2019, doi: 10.1016/j.scitotenv.2019.03.186.

[3] M. Wan et al., “Estimation of soil pH using PXRF spectrometry and Vis-NIR spectroscopy for rapid environmental risk assessment of soil heavy metals,” Process Saf. Environ. Prot., vol. 132, pp. 73–81, 2019, doi: 10.1016/j.psep.2019.09.025.

[4] W. Sun, X. Zhang, X. Sun, Y. Sun, and Y. Cen, “Predicting nickel concentration in soil using reflectance spectroscopy associated with organic matter and clay minerals,” Geoderma, vol. 327, no. April, pp. 25–35, 2018, doi: 10.1016/j.geoderma.2018.04.019.

[5] W. Sun and X. Zhang, “Estimating soil zinc concentrations using reflectance spectroscopy,” Int. J. Appl. Earth Obs. Geoinf., vol. 58, pp. 126–133, 2017, doi: 10.1016/j.jag.2017.01.013.

[6] Y. Yunus, Devianti, P. Satriyo, and A. A. Munawar, “Rapid Prediction of Soil Quality Indices Using Near Infrared Spectroscopy,” in IOP Conference Series: Earth and Environmental Science, Nov. 2019, vol. 365, no. 1, doi: 10.1088/1755-1315/365/1/012043.

[7] D. Devianti, S. Sufardi, Z. Zulfahrizal, and A. A. Munawar, “Rapid and Simultaneous Detection of Hazardous Heavy Metals Contamination in Agricultural Soil Using Infrared Reflectance Spectroscopy,” in IOP Conference Series: Materials Science and Engineering, Apr. 2019, vol. 506, no. 1, doi: 10.1088/1757-899X/506/1/012008.

[8] Darusman, Zulfahrizal, Y. Yunus, and A. A. Munawar, “Soil quality assessment by near infrared spectroscopy: Predicting ph and soil organic carbon,” Int. J. Sci. Technol. Res., vol. 8, no. 10, pp. 2512–2516, 2019.

[9] A. A. Munawar, Y. Yunus, Devianti, and P. Satriyo, “Calibration models database of near infrared spectroscopy to predict agricultural soil fertility properties,” Data Br., vol. 30, Jun. 2020, doi: 10.1016/j.dib.2020.105469.

[10] A. A. Munawar, D. V. Hörsten, D. Mörlein, E. Pawelzik, and J. K. Wegener, “Rapid and non-destructive prediction

of mango sweetness and acidity using near infrared spectroscopy," in Lecture Notes in Informatics (LNI), Proceedings - Series of the Gesellschaft fur Informatik (GI), 2013, vol. P-211, pp. 219–222.
[11] J. Wang, L. Cui, W. Gao, T. Shi, Y. Chen, and Y. Gao, "Prediction of low heavy metal concentrations in agricultural soils using visible and near-infrared reflectance spectroscopy," Geoderma, vol. 216, pp. 1–9, 2014, doi: 10.1016/j.geoderma.2013.10.024.
[12] N. K. N. Che Hassan, M. Taher, and D. Susanti, "Phytochemical constituents and pharmacological properties of Garcinia xanthochymus- a review," Biomed. Pharmacother., vol. 106, no. April, pp. 1378–1389, 2018, doi: 10.1016/j.biopha.2018.07.087.
[13] N. Nakawajana, A. Terdwongworakul, and S. Teerachaichayut, "Minimally destructive assessment of mangosteen translucency based on electrical impedance measurements," J. Food Eng., vol. 171, pp. 137–144, 2016, doi: 10.1016/j.jfoodeng.2015.10.020.
[14] Samadi, S. Wajizah, and A. A. Munawar, "Near infrared spectroscopy (NIRS) data analysis for a rapid and simultaneous prediction of feed nutritive parameters," Data Br., vol. 29, Apr. 2020, doi: 10.1016/j.dib.2020.105211.
[15] Samadi, S. Wajizah, and A. A. Munawar, "Fast and simultaneous prediction of animal feed nutritive values using near infrared reflectance spectroscopy," in IOP Conference Series: Earth and Environmental Science, Mar. 2018, vol. 122, no. 1, doi: 10.1088/1755-1315/122/1/012112.
[16] R. Agustina and A. A. Munawar, "Electro-Optic Properties of Dried Pliek U Powder: Local Ingredients from Aceh," in IOP Conference Series: Earth and Environmental Science, Nov. 2019, vol. 365, no. 1, doi: 10.1088/1755-1315/365/1/012042.
[17] Y. Saputri, Yusriana, and A. A. Munawar, "Infrared spectroscopic features of turmeric powder," in IOP Conference Series: Earth and Environmental Science, Nov. 2019, vol. 365, no. 1, doi: 10.1088/1755-1315/365/1/012051.
[18] A. A. Munawar, H. Syah, and Yusmanizar, "Fast and robust quality assessment of honeys using near infrared spectroscopy," in IOP Conference Series: Earth and Environmental Science, Nov. 2019, vol. 365, no. 1, doi: 10.1088/1755-1315/365/1/012053.
[19] I. Ichwana, Z. Nasution, and A. Arip Munawar, "NEAR-INFRARED SPECTROSCOPY AS A RAPID AND SIMULTANEOUS ASSESSMENT OF AGRICULTURAL GROUNDWATER QUALITY PARAMETERS," INMATEH Agric. Eng., pp. 233–240, Apr. 2020, doi: 10.35633/inmateh-60-26.
[20] R. Hayati, A. A. Munawar, and F. Fachruddin, "Enhanced near infrared spectral data to improve prediction accuracy in determining quality parameters of intact mango," Data Br., p. 105571, Apr. 2020, doi: 10.1016/j.dib.2020.105571.
[21] Agussabti, Rahmaddiansyah, P. Satriyo, and A. A. Munawar, "Data analysis on near infrared spectroscopy as a part of technology adoption for cocoa farmer in Aceh Province, Indonesia," Data Br., vol. 29, Apr. 2020, doi: 10.1016/j.dib.2020.105251.
[22] A. A. Munawar, Kusumiyati, Hafidh, R. Hayati, and D. Wahyuni, "The application of near infrared technology as a rapid and non-destructive method to determine vitamin C content of intact mango fruit," INMATEH - Agric. Eng., vol. 58, no. 2, pp. 1–12, 2019, doi: 10.35633/INMATEH-58-31.
[23] A. A. Munawar, D. von Hörsten, J. K. Wegener, E. Pawelzik, and D. Mörlein, "Rapid and non-destructive prediction of mango quality attributes using Fourier transform near infrared spectroscopy and chemometrics," Eng. Agric. Environ. Food, vol. 9, no. 3, pp. 208–215, Jul. 2016, doi: 10.1016/j.eaef.2015.12.004.
[24] A. A. Munawar, Devianti, P. Satriyo, Syahrul, and Y. Yunus, "Rapid and simultaneous prediction of soil quality attributes using near infrared technology," Int. J. Sci. Technol. Res., vol. 8, no. 9, pp. 725–728, Sep. 2019.
[25] C. D. Iskandar, Zainuddin, and A. A. Munawar, "Beef Freezing Optimization by Means of Planck Model Through Simulation," in IOP Conference Series: Earth and Environmental Science, Nov. 2019, vol. 365, no. 1, doi: 10.1088/1755-1315/365/1/012072.
[26] Sudarjat, Kusumiyati, Hasanuddin, and A. A. Munawar, "Rapid and non-destructive detection of insect infestations on intact mango by means of near infrared spectroscopy," in IOP Conference Series: Earth and Environmental Science, Nov. 2019, vol. 365, no. 1, doi: 10.1088/1755-1315/365/1/012037.
[27] Yusmanizar et al., "Fast and Non-Destructive Prediction of Moisture Content and Chologenic Acid of Intact Coffee Beans Using Near Infrared Reflectance Spectroscopy," in IOP Conference Series: Materials Science and Engineering, Apr. 2019, vol. 506, no. 1, doi: 10.1088/1757-899X/506/1/012033.
[28] R. H. Suci, Zulfahrizal, and A. A. Munawar, "Applying LIBS-QCL spectrum coupled with principal component analysis to distinguish gayo arabica and robusta coffee," Int. J. Sci. Technol. Res., vol. 8, no. 10, pp. 919–924, Oct. 2019.