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Fast and Non-Destructive Prediction of Moisture Content and Chologenic Acid of Intact Coffee Beans Using Near Infrared Reflectance Spectroscopy

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Fast and Non-Destructive Prediction of Moisture Content and Chologenic Acid of Intact Coffee Beans Using Near Infrared Reflectance Spectroscopy

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Abstract. The main objective of this present research is to apply the near infrared reflectance spectroscopy (NIRS) as a fast and non-destructive method in predicting moisture content (MC) and chlorogenic acid (CGA) of intact roasted coffee beans. Diffuse reflectance spectrum were acquired for bulk coffee beans samples (Arabica and Robusta) in wavelength range from 1000 to 2500 nm. Spectra data were corrected and enhanced using standard normal variate (SNV). Prediction models, used to predict MC and CGA of intact coffee beans, were developed and performed using combination of principal component analysis (PCA) and multiple linear regression (PCA+MLR). The results showed that NIRS can be used to predict MC and CGA content of intact coffee beans simultaneously and rapidly with maximum coefficient correlation (r) were 0.92 for MC and 0.93 for CGA, whereas residual predictive deviation (RPD) indexed were 3.67 and 3.87 for MC and CGA content respectively. Based on the obtained results, it may conclude that near infrared spectroscopy can be applied in coffee quality evaluation especially to predict moisture content and chlorogenic acid. NIRS can be used and an alternative fast and non-destructive method bypassing standard laboratory procedures.

Keywords: NIRS; coffee, CGA, Quality; non-destructive

1. Introduction

Coffee is known as famous beverages for people around the worlds due to its taste, flavour and some nutrient content. Interest in coffee quality assessment is impelled by the need to supply the consumer with a consistently high quality product at an affordable price. Indeed, quality is a major aspect for the modern coffee industry because a high quality product is the basis for success in today's particularly competitive market [1]. Moreover, coffee is also one of the most important raw materials within the international trade for which quality is quintessential. Among the several species of the genus coffee identified so far, two of these varieties are economically and commercially important: Coffee Arabica and coffee Robusta. Both coffee varieties differ mutually from a botanical perspective and in terms of quality features [2].

Arabica and Robusta are globally well known and the most traded among those species. Generally, Arabica has gained greater popularity than Robusta. A greater quantity of Arabica is traded and fetches a higher price than Robusta. Differences in prices are also determined by geographical origin. Among



the several species of the genus coffee identified so far, two of these varieties are economically and commercially important [2,3].

Food quality encompasses sensory properties, nutritive values, mechanical properties, functional properties and presence of defects. The majority of traditional techniques used for quality assurance are costly, labour intensive and time consuming, an example being sensory panel evaluation that, to this date, is the ultimate tool to assess coffee quality. Besides being costly and time consuming, sensory panels are inadequate for employment in routine analysis in food processing facilities. In this scenario, infrared spectroscopy is gaining attention since it is capable of solving some of the problems presented by traditional techniques [4].

Moreover, chemical compositions in green coffee beans were used to differentiate between species. Sucrose and trigonelline in Arabica have higher levels than Robusta. Conversely, caffeine and chlorogenic acid (CGA) in Arabica are lower than in Robusta [1,4,5].

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These chemical compositions; caffeine, chlorogenic acid, sucrose, trigonelline are commonly measured by the high-performance liquid chromatography (HPLC). This method has the advantage of being accurate, but, on the other hand, it is time-consuming and needs extensive sample preparation. An alternative to the HPLC is therefore required to provide simplified measurement procedures, specifically for caffeine and chlorogenic acid contents in green coffee beans [8].

In particular, researchers focusing more on Fourier transform infrared (FTIR) and NIR spectroscopy. The FTIR spectrum detects fundamental vibrations in the mid-infrared region ($4000\text{--}400\text{ cm}^{-1}$) whereas the NIR spectrum ($2500\text{--}800\text{ nm}$) arises from the molecular absorptions of overtones and combinations of fundamental vibrational bands in the mid-infrared region. These techniques are rapid, non-destructive and require minimum sample preparation [9,10].

During last few decades, NIRS 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 near to mid infrared region [10, 11].

The feasibility of using infrared spectroscopy in combination with multivariate statistics has been examined with notable success in coffee quality evaluation, with applications including discrimination and quantification of Robusta and Arabica blend, coffee adulteration, and prediction coffee sensory properties [11, 12].

Therefore, the main purpose of this present study is to use the near infrared spectroscopy (NIRS) for coffee quality evaluation in form moisture content (MC) and chlorogenic acid (CGA) content respectively. We develop calibration and prediction models used to predict these both quality parameters simultaneously. We use a combination method of principal component analysis (PCA) and multiple linear regression (MLR) to establish those prediction models.

2. Materials and Methods

2.1. Samples

Green Arabica and Robusta coffee bean samples were collected mainly from Gayo, Aceh Province and some of them were collected from different geographical origins around Indonesia. Coffee samples were taken and stored for three days to equilibrate before spectra acquisition and further chemical analysis were done.

2.2. Diffuse reflectance spectra acquisition

In this study, infrared spectra data of all coffee bean samples were acquired in form of diffuse reflectance spectral data. Background spectra correction was performed every hour automatically. Diffuse reflectance spectra in wavelength range of 1000 – 2500 nm with the increment of 0.2 nm resolution were acquired 64 scans, averaged and recorded in SPA and CSV extension files format [9].

2.3. Moisture content (MC) and Chlorogenic acid (CGA) measurements

Once spectra acquisitions were completed, MC and CGA content for all coffee bean samples were measured using standard laboratory method: Gravimetry for MC measurement and HPLC for CGA content measurement. Both of these actual data were measured in triplicate and averaged.

2.4. Spectra data correction

To enhance and improve prediction performance, spectra correction was employed to all spectra data of coffee bean samples. Standard normal variate (SNV) was chosen as spectra data correction method [9].

2.5. Prediction model performance

Diffuse reflectance spectra data of all coffee bean samples were used to predict MC and CGA content using a combination method of principal component analysis (PCA) and multiple linear regression (MLR). To validate the prediction result, a leverage validation method was applied during prediction 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. It is obvious that good model should have higher R^2 and r coefficient, lower RMSE and RPD above 1.5 [9-12].

3. Result and discussion

3.1. Spectra features of coffee bean samples

Typical Diffuse reflectance spectrum of coffee bean samples in NIR wavelength region range of 1000-2500 nm is shown in figure 1. It corresponds to hydrogen bonds (C-H, N-H, O-H and S-H) and can be used to analyze the chemical composition of organic matter. Additionally, NIR spectra detect the presence of chemical contents that contain hydrogen bonds.

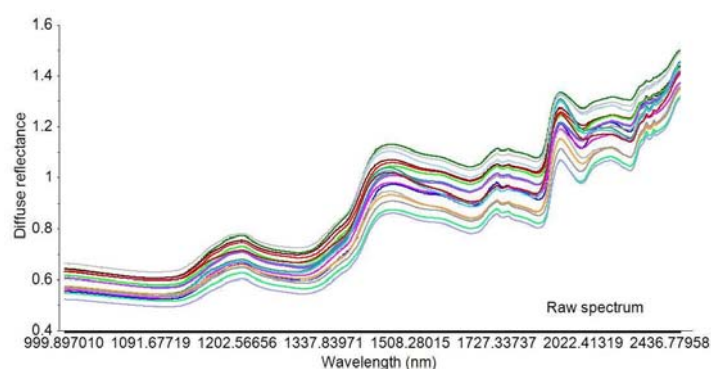


Figure 1. Typical diffuse reflectance spectra data of soil samples before correction.

Infrared spectra data obtained from NIRS instrument, sometimes generally consists irrelevant information and noises due to light scattering. These problems may cause to interfere and affect desired relevant coffee quality attributes such as moisture content and chlorogenic acid content. These noises need to be removed or minimized in order to obtain accurate, robust and stable calibration and prediction

models. Therefore, we employ the SNV spectra correction method before further analysis. Spectra data for all coffee beans samples were corrected and enhanced as presented in figure 2.

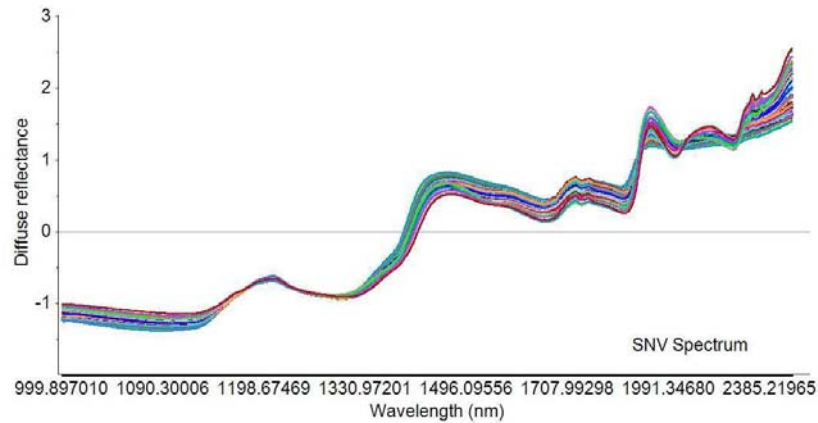


Figure 2. typical diffuse reflectance spectra data of soil samples after SNV correction.

As presented in figure 2, we may see the differences between raw and SNV corrected spectra. Some noises are reduced and we may argue that enhanced spectra may provide and achieve better and accurate prediction results compared to raw un-treated spectra.

After spectra correction was completed, then we attempted to predict MC and CGA content using a combination PCA and LMR regression method with co added of leverage validation. Raw untreated spectra data was firstly employed to predict both MC and CGA content simultaneously. Obtained result shows that MC and CGA content can be predicted better and more accurate using SNV corrected spectra data. Prediction results of MC and CGA in intact coffee bean samples were presented in table 1 and table 2.

Table 1. MC prediction results using raw and SNV spectra data.

Accuracy indicators	Raw spectra	SNV spectra
R^2	0.916	0.975
r	0.938	0.986
RMSE	0.015	0.006
RPD	3.462	4.409

MC: moisture content, R^2 : coefficient of determination, r : correlation coefficient, RMSE: root mean square error, RPD: residual predictive deviation. SNV: standard normal variate.

Table 2. CGA content prediction results using raw and SNV spectra data.

Accuracy indicators	Raw spectra	SNV spectra
R^2	0.512	0.557
r	0.711	0.754
RMSE	1.205	0.936
RPD	1.662	1.960

CGA: chlorogenic acid, R^2 : coefficient of determination, r : correlation coefficient, RMSE: root mean square error, RPD: residual predictive deviation. SNV: standard normal variate.

Maximum correlation coefficient for MC prediction was 0.986 with RPD index of 4.409, which indicated as an excellent prediction model. On the other hand, CGA prediction results was categorized as coarse sufficient model since the maximum correlation coefficient between predicted and reference

CGA data was 0.754 and RPD index was 1.960. Scatter plot derived from reference and predicted quality parameters (MC and CGA) are shown in figure 3 and figure 4.

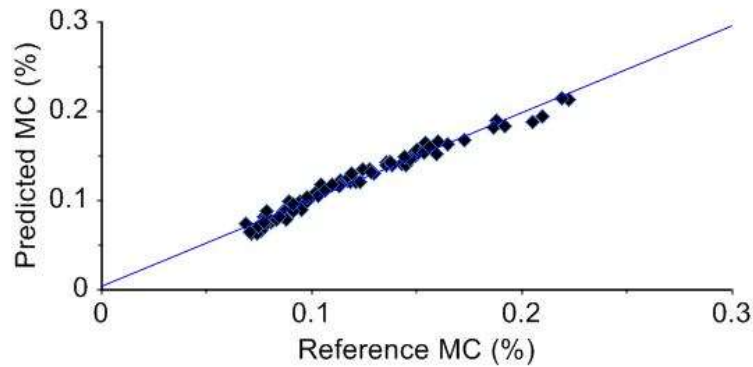


Figure 3. Scatter plot of reference versus predicted moisture content (MC) based on SNV spectra.

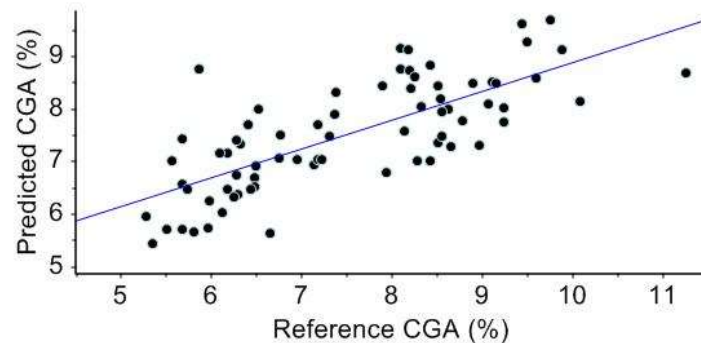


Figure 4. Scatter plot of reference versus predicted chlorogenic acid (CGA) based on SNV spectra.

Furthermore, we found on this study that MC and CGA of intact coffee bean samples can be predicted better when SNV spectra was used. Thus, we may argue that spectra data need to be enhanced and improved before further analysis. This also in agreement with some other researchers [13, 14, 15]. However, further enhancement must be conducted to increase and improve prediction accuracy. This enhancement can either adding the number of samples to be involved, or applying combination spectra enhancement method such as a combination of SNV correction method and other correction such as multiplicative scatter correction (MSC) and baseline shift correction (BSC).

4. Conclusion

Based on achieved results, we may conclude that near infrared spectroscopy (NIRS) can be used to predict moisture content (MC) and chlorogenic acid (CGA) content of intact coffee bean samples. Achieved results, shows that MC can be predicted with maximum correlation coefficient is 0.98 and residual predictive deviation (RPD) index is 4.41 with categorized as excellent result. However, CGA can be predicted sufficiently using enhanced spectra with maximum correlation coefficient of 0.75 and RPD index of 1.96. Further spectra data analysis and non-linear regression approach may be applied to enhance accuracy and prediction robustness.

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