Non-destructive Evaluation of Fat Content of Coffee Beans Solok Radjo Using Near Infrared Spectroscopy

F Yuwita¹, Ifmalinda² and M Makky²
¹Magister Student of Biosystem and Bioproses Engineering, Andalas University, Padang, Indonesia,
²Department of Agricultural Engineering, Andalas University, Kampus UNAND Limau Manis Padang 25163 West Sumatera, Indonesia

Corresponding author’s e-mail address: fitriyuwita.s@gmail.com

Abstract. Prediction fat of coffee beans in West Sumatra is still done manually by chemical methods, time-consuming, and costly. With the development of food technology, the estimation of the content of the beans to do with how quickly and efficiently using NIRS technology. NIRS can analyze the chemical content of foodstuffs nondestructive. This study uses Arabica beans Solok Radjo two maturity levels are 4 (ripe) and 5 (over ripe), 30 samples with weight of samples 6 grams. NIRS instrument used is the science and technology FT-IR-1516 with a wavelength of 1000-2500 nm. Fat tests conducted in the laboratory Instrumentation Technology Center for Agriculture. In this study, the data spectral coffee beans processed using PCA (Principal Component Analysis) after correlated with fat content processed by the method of PLS (Partial Least Square). The prediction results of calibration best fat obtained \( r = 0.999, R^2 = 0.999, \text{SEC} = 0.008\% \), and RMSEC = 0.008\%, validating the value of \( r = 0.998, R^2 = 0.999, \text{SEP} = 0.009\% \), and RMSEP = 0.008\%, of the model fat coffee beans can be identified by non-destructive evaluation using spectral analysis.

1. Introduction
Indonesia is known as one of the coffee producing countries and the world's largest exporter of coffee beans. West Sumatra in 2015 produces coffee as 34.059 tons of coffee, with planting areas of 42.925 Ha [4]. One of the producing coffee in West Sumatra is distric of Solok, famous with coffee names Minang Solok Radjo. Solok Radjo coffee at the moment it feels have been identified in Indonesia and Abroad, Solok Radjo coffee in 2016 becomes the winner and get the highest score in West Sumatra coffee festival as a quality coffee speciality, this was proved in 2013 the coffee was exported to the United States have as much as 4 ton, Australia 22 tons, to Italy 2 tons and 1.5 tons to Thailand [4].

Postharvest handling is key to success to improve the quality of Indonesian coffee beans. The estimation of the quality of the coffee is usually done through laboratory testing (destructive), where coffee beans are crushed and the juice is taken and analyzed by standard methods of chemical common in laboratories. However, the chemical method to spend a long time and cost a fortune, so it is not suitable to be applied in industries that require a very fast method and not destructive (non-destructive) to analyze the quality of the coffee. The detection of food quality can be realized quickly and
efficiently through technological development Nir Spectrometer (NIRS). NIRS can be analyzed more quickly does not use chemicals and can analyze the chemical content of materials without damage.

Some research has been done before, as it has done [7], which analyzed the caffeine content of coffee powder. The results showed the caffeine content of coffee 6% higher when compared with UV detection. LC-UV method selected as the reference method for the calibration of NIRS system. Analysis on 83 samples of liquid coffee extract resulted in SEE (standard error of estimate) 0.34% while for SEP (standard error of prediction) of 0.07% with a correlation coefficient of 0.86. [14] has also been conducting research NIRS to predict that whole coffee beans caffeine content Gayo Arabica coffee beans, according to the determination of the chemical composition of coffee more efficiently and effectively carried out in the form of coffee beans than coffee powder.

The use of NIRS has many advantages compared to traditional testing is a simple preparation of samples, can analyze samples in the form of powder and seeds, rapid detection process, do not use chemicals. NIRS research on coffee has much to do but have not been to a coffee Minang Solok Radjo because Indonesia has a wide range of coffee varieties that have different characteristics. Therefore, the development of NIRS research with the object of coffee Solok Radjo need to be supported and developed to facilitate detection of the chemical content of the coffee beans quickly and accurately.

2. Materials and Methods
In this study, the samples’ fat is determined through electromagnetic radiation absorbance, measured using NIR spectroscopy. 1 kg grams of coffee beans Solok Radjo with two maturity they are maturity level 4 (ripe) and maturity lever 5 (overripe) were harvested by manual picking from the stem. The beans were cleaned and placed into 30 ml glass tubes. The samples were compacted by placing the tubes on vortex for 10 seconds. More beans were added and procedure repeated until the tubes were fully filled. The sample’s tubes were then placed into NIR spectroscopy and its spectral (1000-2500 nm) were recorded at normal scan speed using average of 10 scans method. Recorded signals were pre-processed with spectroscopy software (Unscrambler® X.1, Camo, USA).

The measured actual samples’ fat by primary method [1]. As many 3 grams of sample (W0) is inserted into a filter paper that had been closed both ends with fat free cotton and inserted into the fatty sheath that has measured its permanent weight (W1) and connected with the soxhlet tube. Fatty sheath tube inserted into the soxhlet extractor chamber and added fat solvent (n-hexane). Then the solution at reflux for 3 hours. Solvents fat in the fat flask was distilled until all the fat solvent evaporated. Furthermore, fat tube dried in an oven at a temperature of 105 °C and tube dried in the desiccator until its weight is constant (W2). The calculation of fat content can use the formula:

\[
\text{Fat (\%)} = \frac{W_2 - W_1}{W_0} \times 100\% 
\]

where W0 is weight of samples (g), W1 is weight empty fat tube (g), W2 is weight tube with fat (g).

The absorbance data was then analyzed using software (Unscrambler® X.1, Camo, USA) to correlate with its fat. PCA method was used to identify significant correlation between certain electromagnetic radiation wavelengths with sample’s fat. Model to determine fat of the samples according to its electromagnetic radiation absorbance was developed using PLS, were in maturity level 4 using pretreatment normalization. Pretreatment normalization method is part of the normalization obtained by dividing each row of the matrix of data averaging so as to reduce the interference of factors that are not visible [6].

The samples fat as dependent variables, and the PCs from PCA analysis as factors. Data was partitioned into two groups; the first 2/3 (20 data) was used to train the model, and the rest of 1/3 (10 data) was used to validate the model. Model performance was analyzed using Sum of Squares Error (SSE), and Relative Error (RE).

3. Results and Discussion

3.1. NIRS spectrum and Chemical Ingredients Raw Coffee Beans Solok Radjo
Spectrum raw NIRS is a raw spectrum from the data given NIRS without pretreatment, from raw spectra can find the amount of noise generated and to know the chemical constituents in the beans. Chemical content indicated by the peaks and valleys of the resulting wavelengths on the spectrum. NIRS spectrum of the raw coffee beans are Arabica Solok Radjo between 1000-2500 nm wavelength can be seen in Figure 1.

![Figure 1. Raw NIRS Spectrum Arabica Coffee Solok Radjo.](image)

Coffee beans spectrum has peaks and valleys at a particular wavelength, peak spectral absorbance NIRS in Solok Radjo Arabica coffee beans is between wavelengths 1128-1140 nm, 1202-1221 nm, 1392-1418 nm, and 1731-1766 nm, it shows information where the content of certain substances found in coffee. This is in accordance with the opinion [2], that the chemical components contained in the material to be tested affect the existence of the peaks and valleys of the spectrum, in addition to the peaks and valleys of the spectrum is also influenced by the physical properties of the material to be analysed.

3.2. NIRS spectrum classification Solok Radjo Coffee Beans on Two Levels Maturity
Classification of two coffee beans Solok maturity level Radjo seen by taking each of the spectrum of maturity level 4 (ripe) and 5 (overripe), this is to look at the differences of each spectrum. The results of the classification of spectrum of coffee beans in the maturity level 4 (perfectly cooked) and 5 (overripe) can be seen in Figure 2.

![Figure 2. Classification of NIRS Spectrum of Solok Radjo Coffee Beans](image)
Figure 2 show of spectrum results indicate that the spectrum of a typical coffee bean has the same pattern, but has a absorbance absorption values were somewhat different, this is due at the time of data collection is still no light is passed out materials as well as the difference of the chemical component contained by coffee. [12] said that the difference in the spectrum caused by several kinds disorders like rays of light from the sample, the difference in temperature, density and particle size and other disturbances coming from the detector, AD converter, or amplifier.

Analysis to see the difference in the maturity level of the coffee beans Solok Radjo using PCA (Principal Component Analysis). Conduct an analysis of factors to get a new variable in smaller amounts, PCA can be used as a basis [8]. PCA analysis performed to determine whether the maturity of the beans can be directly distinguished from each other. [10] states that the PCA is able classify an appropriately different materials such as classifying according to its kind. The results of PCA analysis Solok Radjo coffee beans can be seen in Figure 3.

![Figure 3. Results of PCA Analysis NIRS Solok Radjo Coffee Beans](image)

The results of PCA analysis on raw (original data) coffee beans without pretreatment spectrum as shown in Figure 3, shows that they are separated or grouped well. Coffee beans in the maturity level 4 (ripe) are in the same pile as well as coffee beans at maturity level 5 (overripe). PCA can prove the difference spectrum at each maturity level Solok Radjo coffee beans. PCA results prove that NIRS can segment data based on the maturity level of the coffee beans. This shows the spectrum of coffee beans can be classified as good with a percentage of 100% success. Wavelength NIRS measurement results that are relevant to determining the substance content in coffee Solok Radjo show in Figure 4.

![Figure 4. The Relevant Wavelength Solok Radjo of Coffee Beans](image)
The result of the loading of the plot on raw coffee bean Solok Radjo spectrum shows the presence of peaks and valleys that indicates the presence of chemical substances content in the coffee. Based on the analysis of spectral peaks based on the description information table Cen and He [3] the fat is located at a wavelength of 1379-1388 nm, 1720-1733 nm, and 2300-2346 nm.

3.3. Prediction Model Calibration and Validation Results Fat Content Coffee Beans Solok Radjo Using PLS (Partial Least Squares Regression) Method.

Calibration and validation of coffee Solok Radjo models using software Unscramble X.1 with Partial Least Square Regression method. PLS is a relatively new approach to linear regression and algorithms. PLS calibration suitable for incorporation in a number of samples with chemical data destructively tested in the laboratory and data NIRS [16]. Model calibration is the relationship between the data absorbance NIRS and chemical data coffee Solok Radjo, the model calibration are well defined with parameters SEC, SEP, Bias, the difference in value of the SEC with the SEP, the correlation coefficient between the actual value and the predicted number of factors or variables latent etc. [9].

The fat content in Arabica coffee contained in a protective wax coating on oil seeds and coffee. Fat in coffee is one of the chemical composition of coffee shape coffee flavor. Total fat content in arabica coffee between 12-18% which is contained in a layer of protective wax beans [15]. The increase in free fatty acids during storage will cause rancidity in the coffee powder so that it will affect the taste and the quality of the coffee powder. [13] fat content is marked by a chain of chemical bonds CH.

Fat content prediction data processing coffee beans for two different maturity levels using methods Partial Least Squares Regression (PLS) can be seen in Figures 5a and 5b.

Results of the PLS prediction estimation can be seen from the results of the SEC and SEP error values obtained are still small, The resulting high r value, and the value of the error (RMSEC and RMSEP) is small, [16] is said to have good models when the error value generated RMSEC smaller than the standard deviation of the actual data. The results of the calibration predictive value $r = 0.999$, $R^2 = 0.999$, SEC = 0.008%, and RMSEC = 0. 0.008%, while the yield for the validation of the value of $r = 0.998$, $R^2 = 0999$, SEP = 0.009%, and RMSEP = 0.008%. [11] states that the determination value above 0.91 can be said to be good models. Use of PLS can predict the fat content of the coffee beans in the maturity level 4.

Spectral data processing coffee beans Solok Radjo at maturity level 5 (overripe) can be seen in Figure 6.
Figure 6a. PLS model calibration for samples’ fat content coffee beans Solok Radjo at maturity level 5 (overripe)

Figure 6b. PLS model validation for samples’ fat content coffee beans Solok Radjo at maturity level 5 (overripe)

Figure 6 shows the results of a plot of data calibration and validation fat coffee beans Solok Radjo which were obtained by the predictive value of the calibration is $r = 0.999$, $R^2 = 0.999$, SEC = 0.003%, and RMSEC = 0.003%, while for validation is $r = 0.999$, $R^2 = 0.998$, SEP = 0.072%, and RMSEP = 0.062%. The results of PLS estimation without the fat content of coffee beans to show that the value of $r$ obtained is big enough that that is above 0.91 and for the error value (RMSEC and RMSEP) obtained good report because less than zero.

4. Conclusion
In this study, nondestructive methods can be used to test the fat content of the coffee beans Solok Radjo. Model with absorbance values that are absorbed from the beans by using PLS. NIRS spectrum wavelength used is 1000-2500 nm and fat Solok Radjo arabica coffee is at a wavelength 1379-1388 nm, 1720-1733 nm, and 2300-2346 nm. Upon validation the model obtained value $R^2 = 0.999$ and RMSEP = 0.008%. Conclusion this research, NIRS can be used to estimate the fat content of coffee beans and as information for merchants to increase the quality of the coffee beans that will be marketed.

References
[1] AOAC International 1995 *Official Methods of Analysis of AOAC International* AOAC International. Secs. 942.15. Washington USA
[2] Blanco M and Villarroya I 2002 *NIR spectroscopy a rapid-response analytical tool* Trends in analytical chemistry 21 240-250
[3] Cen H, and He Y 2007 *Theory and application of near infrared reflectance spectroscopy in determination of food quality* J. Trends in Food Sci & Technol 18 72-83
[4] Directorate General of Plantation. 2016. *Statistics Indonesia Plantation* Jakarta
[5] Fajarudin 2016 *Will be Solok Coffee Export 18 Tons* The bow May 6 Padang
[6] Gaydow V, Kister J, Dupuy N 2011 *Evaluation of multiblock NIR / MIR PLS predictive models to detect adulteration of diesel / biodiesel blends by vegetal oil* Journal of Chemometrics and Intelligent Laboratory Systems 106 190-197
[7] Huck C W, W Guggenbichler GK Bonn 2005 *Analysis of caffeine, theobromine and theophylline in coffee by near infrared spectroscopy (NIRS) compared to high-performance liquid chromatography (HPLC) coupled to mass spectrometry* J Analytica Chimica Acta 538 195-203
[8] Iriawan N and Astuti S P 2006 *Statistics Data Processing with Easy to Use Minitab 14* Yogyakarta (ID) Andi
[9] Lammertyn J, Peirs A, De Baerdemaeker J and Nicolai B M 2000 *Light Penetration Properties of NIR Radiation in Fruit with Respect to Non-Destructive Quality Assessment* J Postharvest Biol Technology 18 121-132

[10] Lee V S, Tue-Ngeun P, Traisathit P, Prasitwattanaseree S, Nimmanpipug P and Chaijaruwanich J 2009 *FTNIR and chemometric tools for the classification of thai wines*. Journal of Science and Technology 3 446-458

[11] Mouazen A M, Saeys W, Xing J, De Baerdemaeker J and Ramon H 2005 *Near infrared spectroscopy for agricultural materials: an instrument comparison a near infrared spectroscopy* 13 87-97

[12] Ozaki Y, McClure W F and Christy A A 2007 *Near-Infrared spectroscopy in food science and technology* New Jersey (USA) John Wiley & Sons, Inc

[13] Rita H, Marlihia A and Rosita F 2011 *Study of Three Varieties and Two Against Fermentation Method Quality Arabica coffee beans (Coffea arabica L.) Gayo, Bener Rousing* Proceedings of the Seminar The National Association of Expert Food Technology Indonesia (PATPI) North Sumatra

[14] Rosita R 2016 *Determination of chemical constituents Gayo Arabica coffee beans are non-destructively by near infrared spectroscopy* [Thesis] Bogor Graduate School of Bogor Agricultural University

[15] Wei F and Tanokura M 2015 *chemical change in the components of coffee beans during roasting* J Health and Disease Doi.org/10.1016/B978. 12 409-517

[16] Williams P and Norris K 1990 *Near-infrared technology in the agricultural and food industries*. American Association of cereal chemical, Inc. St. Paul USA 146