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Research Article

The Utilization of Ftir (Fourier Transform Infra-Red) Method Combined with Chemometrics For Authentication of Indonesian Coffee Powder

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ABSTRACT

Analysis of natural product remain challenging issues for analytical chemist, since natural products are complicated system of mixture. The most popular methods of choice used for quality control of raw material and finished product are high performance liquid chromatography (HPLC), gas chromatography (GC) and mass spectrometry (MS). The utilization of FTIR-ATR (Fourier Transform Infrared-Attenuated Total Reflectance) method in natural product analysis is still limited. This study attempts to expand the use of FTIR spectroscopy in authenticating Indonesian coffee powder.The coffee samples studied were taken from nine regions in Indonesia, namely Aceh Gayo, Flores, Kintamani, Mandheling, Papua, Sidikalang, Toraja, Kerinci and Lampung.The samples in the form of coffee bean from various regions were powdered . The next step conducted was to determine the spectrum using the FTIR-ATR (Attenuated Total Reflectance) using ZnSe crystal of 8000 resolution. Spectrum samples, then, were analyzed using chemometrics. The utilized chemometric model was the principal component analysis (PCA) and cluster analysis (CA). Based on the chemometric analysis, there are similarities between Aceh Gayo coffee with Toraja coffee, Mandailing coffee, Kintamani coffee and Flores coffee. Sidikalang coffee has a similarity to Flores coffee; Papua coffee has a similarity to Sidikalang coffee; Lampung coffee has a similarity to Sidikalang coffee, while Kerinci coffee has a similarity to Papua coffee.

Keywords: Coffee Powder, Spectrophotometer FTIR-ATR, Authentication, Chemometrics.

INTRODUCTION

Coffee is one of the results of the agricultural commodity having economic value which is high enough among other plantation crops and plays an important role as a source of foreign exchange. Coffee not only plays an important role as a source of foreign exchange but also becomes a source of income for no less than one and a half million coffee farmers at different region in Indonesia[1]. Natural product including plants undergoes natural variation. The quality of samples from different localities and growing condition based on their geographical origin may vary. Thus, the identification of crude samples based on geographical origin is crucial in order to ensure authenticity and quality of the raw material before it is converted to final product[2]. The authentication could be done by LCMS (Liquid Chromatography Mass Spectroscopy) method and GCMS. Unfortunately, both methods require complicated sample preparation and time-consuming implementation. In addition, the method employing many reagents are not environtmentally friendly[3]. Based on this, more practical methods of analysis are required. In this case, Fourier transform infrared spectroscopy is the preferred method used. This is due to some of the benefits of its usage, namely simple operation, faster time analysis and environmentally friendly because of its little usage of reagents.

The FTIR (Fourier Transform Infrared) Spectrophotometry is infrared spectroscopy equipped with the Fourier transform for detecting and analyzing the results of its spectrum. The analysis using FTIR has been conducted for curcumin analysis which is generally performed using thin-layer chromatography method[4,5,6] or high performance liquid chromatography[8,9]. In this study FTIR (Fourier Transform Infrared) spectrophotometry, which is combined with chemometrics,will be applied to authenticate the coffee. The chemometrics model used are Principal Component Analysis (PCA) and Cluster Analysis (CA)[3,10].

MATERIALS AND METHOD

Equipment

Equipment used in this study includes FTIR Spectrophotometer (Therno Scientific Nicolet iS5), pH meter (MettlerTeledo), moisture balance (Precisa Gravimetrics AG / Switzerland).

Material

Materials used are coffee beans and distilled water.

Sample Preparation

The preparation of test samples conducted in stages starts from roasting, grinding, and sieving.

Determination of Coffee Specifications

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Table 1: The result of the coffee drying shrinkage measurement.

Num	Coffee	Initial weight (gram)	Result of drying shringkage (%)
1	Aceh Gayo Arabica	1	6.95
2	Flores Arabica	1	7.75
3	Kintamani Arabica	1	7.73
4	Mandailing Arabica	1	7.83
5	Papua Arabica	1	7.20
6	Sidikalang Arabica	1	7.25
7	Toraja Arabica	1	7.78
8	Kerinci Robusta	1	7.89
9	Lampung Robusta	1	7.45

Table 2: The result of coffee-solubility measurement.

Num	Coffee	Solubility of coffee (%)	
		At 25 ^{o}C	At 80^{o}C
1	Aceh Gayo Arabica	14.62	17.84
2	Flores Arabica	16.9	15.54
3	Kintamani Arabica	18.16	20.6
4	Mandailing Arabica	15.14	24.1
5	Papua Arabica	17.74	20
6	Sidikalang Arabica	15.58	22.2
7	Toraja Arabica	16.04	23.34
8	Kerinci Robusta	17.96	23.96
9	Lampung Robusta	16.86	22.06

Table 3: Result of pH measurement.

Num	Coffee	pH
1	Aceh Gayo Arabica	4,79
2	Flores Arabica	5,09
3	Kintamani Arabica	4,73
4	Mandailing Arabica	4,77
5	Papua Arabica	4,99
6	Sidikalang Arabica	4,82
7	Toraja Arabica	4,82
8	Kerinci Robusta	5,17
9	Lampung Robusta	5,22

The coffee specidications determination includes coffee particle size uniformity test, drying shrinkage, coffee solubility, and acidity or pH measurement.

Coffee powder particle size uniformity

The uniformity of the particle size was conducted by sieving using a mesh number 80, aiming to get finer coffee powder for FTIR test.

Drying shrinkage

Determination of drying shrinkage was conducted by weighing as much as 1 gram of powdered coffee, placed into moisture balance equipment, a triple treatment was conducted.

Coffee solubility

Coffee solubility measurements was conducted in accordance with SNI 2983:2014 regarding instant coffee. From the results of the brewed coffee, the percentage amount of dissolved coffee was calculated.

Acidity or pH measurement

Measuring the degree of acidity or pH could be done by using a pH meter which has been calibrated. Coffee powder had been dissolved in hot water; after it was cold, the acidity on the steeping of the coffee powder was measured. Measurements were made as many as three times.

Determination of the main FTIR spectrum of the test sample

Analysis of coffee powder was conducted using FTIR spectrophotometer at the range of wavenumber 4000-500 cm^{-1}. Each test sample was determined by the method of ATR (Attenuated Total Reflectance) using ZnSe crystal with the resolution of 8000. Then, the manipulation of the spectrum was conducted by smoothing 9 (17.356 cm^{-1}) to each of the resulted spectra.

Chemometric spectrum analysis

Each resulted spectrum was analyzed using chemometrics with principal component analysis (PCA) and cluster analysis (CA) based on the similarity. Each absorbance spectrum data was obtained with a different wave number. The absorbance at 15 wave number (800-3800 cm-1) value data were analyzed by chemometrics using Minitab Software.

RESULT AND DISCUSSION

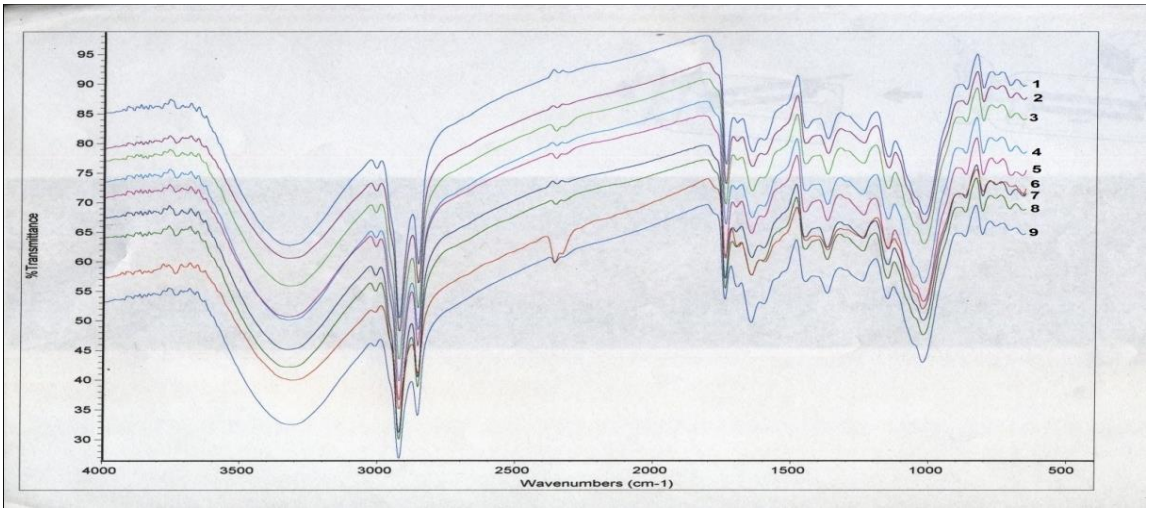

Figure 1: The result of FTIR Spectrum determination of coffee powder . 1. Aceh gayo ; 2.Flores;3.Kintamani; 4.Mandailing; 5.Papua; 6.Sidikalang; 7.Toraja; 8.Kerinci; 9.Lampung.

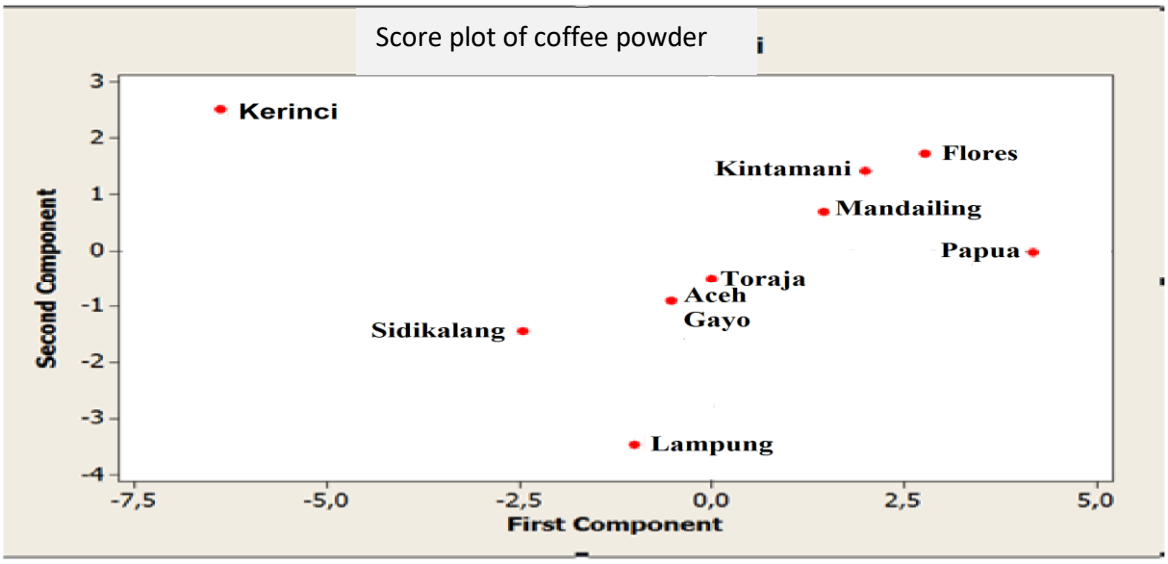

Figure 2: The result of PCA analysis.

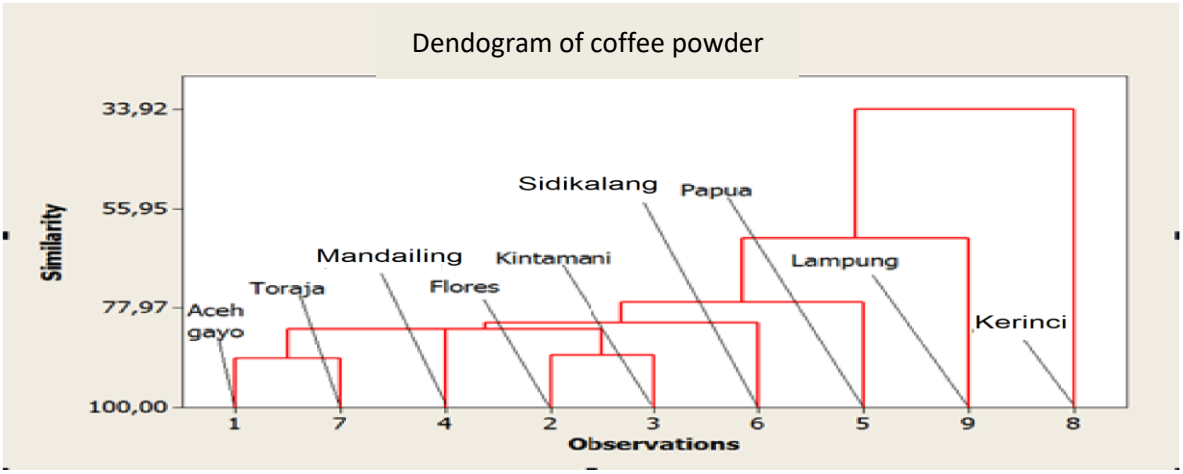

Figure 3: The result of Cluster Analysis of coffee powder.

From the result of organoleptic test which includes seed shape, color and texture between Arabica and Robusta coffee,a difference of colors and shapes before grinding can be observed, yet after all the types of coffee were ground, they could not be distinguished because almost all of the types of coffee have the same color and odor.

The result of Drying shrinkage, coffee solubility, and pH measurement were tabulated in table1,2, and 3. Based on table-1, after all of the types of coffee was heated at the temperature of 115^0C for 60 minutes, the obtained values indicate that the Aceh Gayo coffee has the smallest shrinkage value compared to others. According to the table- 2, it can be seen that at the temperature of 25^0C, Kintamani coffee has the greatest solubility than others, while Aceh Gayo coffee has the lowest solubility of all. However, at a temperature of 80^0C. Mandailing coffee has the greatest solubility,yet Flores coffee has the lowest solubility.

From the data in table-3 it can be seen that the coffee having the highest degree of acidity is found in the Kintamani coffee, and Lampung coffee has the lowest degree of acidity.

The result of spectrum determination of ground coffee beans, can be seen in figure 1. For all of the spectrums, spectrum manipulation was conducted for reducing the spectrum of wave number which was too close together since almost all of the obtained spectrum results have a similarity which is difficult to distinguish from one and another. Therefore, there should be further analysis of the spectrum results using chemometric methods. Principal component analysis (PCA) and cluster analysis (CA) are conducted by collecting all the data absorbance of each coffee with some wave numbers. The result of PCA shown in figure 2. The result of principal component analysis (PCA) produced a score plot. The distance of the points on the score plot shows the closeness between each coffee. The obtained data through principal component analysis (PCA) using chemometrics can show the closeness among all types of the studied coffee. The analysis using principal component analysis or (PCA) is a little disconcerting to grasp the similarity between each coffee because of some distant point and adjacent. Therefore, to ensure and understand the similarity of each coffee, it is necessary to conduct cluster analysis.

The results of the analysis using CA in the form dendrogram show the similarity percentage between each coffee. The greater the similarity percentage, the more similarities owned by the coffee.The results of cluster analysis can be seen in Figure 3. From the obtained dendrogram result in the picture, the similarity between each coffee can be seen.

From this study, it was proved that FTIR spectrophotometry method combined with chemometric model of PCA (Principal Component Analysis) and CA (Cluster Analysis) has successfully authenticated coffee samples obtained from nine different regions in Indonesia, namely Aceh Gayocoffee, Florescoffee, Kintamani coffee, Mandailaing coffee, Papua coffee, Sidikalang coffee, Toraja coffee,Kerinci coffee,and Lampung coffee.

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