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Non-Invasive NIR Spectroscopy for Precise Water Content Determination in Sumatran Coffee Beans

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ABSTRACT

The amount of water in roasted coffee beans can lead to fat oxidation, shortening their shelf life and affecting both the grinding procedure and the distribution of particle sizes in the coffee powder. In this work, the ability of NIR spectroscopy to ascertain the water content of Sumatran-roasted coffee beans will be evaluated non-invasively. The Thermo Nicolet Antaris TM II NIRS device collected NIR spectrum data for wavelengths between 1000 and 2500 nm, which has a high response to water content. The reference water content is calculated using the gravimetric method. Pre-processing techniques used to generate the calibration model include multiplicative scatter correction (MSC) to eliminate optical path differences, the Savitzky-Golay 9-point smoothing window, first-order derivative (SG-1stD) to smooth the spectra, and a combination of MSC and SG-1stD (MSC+SG-1stD). According to research findings, the calibration model employing the MSC+SG-1stD pre-processing techniques provides the most accurate prediction of the water content of Sumatran roasted coffee beans with Rp^2 = 0.995 and RMSEP = 0.003%. This finding will significantly impact the coffee industry, guarantee high-quality roasted coffee beans, and increase competitiveness in international markets. This is due to the ability of the NIR spectroscopy method to provide water content results quickly compared to conventional methods that require a relatively long time to carry out measurements, even though it gives accurate results if done carefully and using well-calibrated equipment. Additionally, this study advances our understanding of how to use NIR spectroscopy to evaluate roasted coffee quality and extends its applicability to Sumatran coffee, which is renowned for its distinctive qualities.

1. INTRODUCTION

Water content is one of the factors that influences the quality of a food product, including roasted coffee beans. The water content of roasted coffee beans can increase during storage because of their porous structure and reduced density [1], making them very hygroscopic [2]. Moreover, the water content exceeding 5% in roasted coffee beans can trigger fat oxidation, shortening coffee's shelf life [3]. It regulates retention and maintains aroma stability during storage [4]. Also, grinding coffee beans with a water content exceeding 6% can produce an unsatisfactory particle size distribution [5].

Sumatran coffee beans, including them, are among the seven characteristics of Indonesian coffee. The diversity of characteristics of Indonesian coffee cannot be separated from Indonesia's geographic location, which is located in the coffee production zone known as the "bean belt." One of Sumatran coffee's geographical characteristics is its climate. Climate differences impact air humidity and the coffee bean drying process, which affects coffee beans' water content.

Furthermore, the water content of Sumatran coffee beans determines the roasting process. Even though the water content of Sumatran coffee beans does not yet have a definite standard, coffee beans with high water content, under light roasting, develop a complex and smooth flavor and maintain the acidic characteristics of coffee beans. Meanwhile, coffee beans with a low water content use dark roasting to produce a heavier flavor. Indirectly, the water content determines the unique flavor characteristics of Sumatran-roasted coffee beans. Therefore, measuring the water content is crucial to ensure coffee beans roasted meet quality standards and increase their competitiveness in the global market.

Analytical methods for measuring coffee bean moisture content include oven drying and Karl-Fischer titration [6]. There are three ISO standards for measuring water content: ISO 1446, 1447, and 6673 [6, 7]. This method is time-consuming, especially the Karl-Fischer titration method, which requires chemical analysis. NIR spectroscopy can perform analysis relatively quickly with simple sample preparation, does not require chemicals, and tests without damaging the product, thereby maintaining the integrity of food ingredients. In addition, combining NIR spectroscopy with chemometrics is common and has been widely used to determine coffee beans' chemical composition and quality attributes.

For coffee beans, NIR spectroscopy has been used in several prior research in diverse contexts, including prediction of the color of the roast and other aspects of the coffee's quality [8]; prediction of coffee roasting degree [1, 9]; measurement of the roasting level and the Arabica/Robusta ratio in roasted and ground coffee at the same time [10]; rapid prediction of intact green coffee beans' moisture content [11]; rapid estimation of the moisture and lipid content of a single green coffee bean using hyperspectral imaging [12]; identifying the sensory characteristics induced by professional coffee cupping [13]; description of unroasted, roasted, and ground coffee [14]; predicting the electric conductivity and potassium leaching of coffee [15]; authentication of Gourmet ground roasted coffees [16]; and the monitoring of moisture content in roasted and ground coffee [5]. Despite all the studies mentioned above, only a few publications have investigated the moisture content of roasted coffee beans and have only focused on evaluating the water content of roasted coffee beans of Arabica and Robusta species grown in the Brazilian states of Espírito Santo, Minas Gerais, and Paraná. Although both involve coffee bean processing processes such as roasting, geographic origin also impacts the final characteristics of the coffee bean product [17].

The development of a calibration model using the NIR spectroscopy method to predict the water content of Sumatran roasted coffee beans remains incomplete. Our research determined that Sumatran roasted coffee beans have different characteristic spectral patterns in the NIR wavelength region that are strongly influenced by water content as a result of different geographical factors. We explicitly state that measuring the water content of Sumatran roasted coffee beans using NIR spectroscopy has implications for coffee industry practice, where one of the benefits for coffee producers is being able to avoid losses due to incorrect water content in storage and shipping.

Furthermore, we emphasize the importance of our work because it can provide convenience and speed in non-destructive measurement of water content, thereby increasing efficiency and accuracy in analyzing the quality of Sumatran roasted coffee beans. We also state that our work contributes to additional literature in the field of coffee postharvest. Therefore, it is essential to evaluate the water content of Sumatran roasted coffee beans using NIR spectroscopy by considering these geographical differences.

Our study aimed to evaluate the potentiality of the NIR spectrum to estimate the moisture content of Sumatran-roasted coffee beans. Furthermore, we hypothesized that the NIR spectrum could be a dependable indicator for predicting water content in Sumatran roasted coffee beans.

2. MATERIALS AND METHODS

2.1 Coffee bean samples

Fifty-four green coffee bean samples in total were gathered from Sumatra, Indonesia's diverse coffee-producing regions, including Aceh (n = 10), West Sumatra (n = 18), South Sumatra (n = 18), and Lampung (n = 8).

2.2 Water content analysis

The reference water content in roasted coffee beans was measured using the thermogravimetric method according to ISO 6673 standards. It is internationally recognized for its precision and reliability in measuring and determining water content, especially in our coffee sample matrix. Its application is well documented in peer reviewed literature, offering a robust framework for our analytical procedures. Moreover, the method is specifically designed to minimize the potential for errors associated with other techniques, such as those that might arise from volatile substances other than water. Approximately 10 grams of roasted coffee beans were dried in an open glass petri dish with a Thermicon type UT6120 instrument (Heraeus Instruments GmbH, Hanau, Germany) at 105 ± 1°C for 16 hours. After drying, the sample was placed in a desiccator for 1 hour to cool to room temperature. In order to determine the water content based on mass change, the sample was finally weighed (Type LP 620 S, Sartorius AG, Göttingen, Germany).

2.3 NIR spectrum collection

Using a NIRS Thermo Nicolet Antaris TM II instrument, the NIR spectra of a batch of 50 g of coffee beans were collected by a wavelength scanning process of 1000–2500 nm with an increment interval of 2 nm. Background or reference calibration is done every hour to keep the sensor stable. The outcomes of measuring the diffuse reflectance spectrum on roasted coffee bean samples are realized.

2.4 Spectral pretreatment

When scanned, Sumatran roasted coffee beans will most likely create spectra that contain background information or interference from gaps between coffee beans in addition to the chemical information of the sample. Because Sumatran roasted coffee beans often have a low water content, extra pre-processing in the form of derivatives is required to enhance the peak signal in the NIR absorption spectrum. As a result, we decided to use the Multiplicative Scatter Correction (MSC) approach during pre-processing. The MSC method can reduce the effect of scattered light thoughts and changes in NIR spectrum transmission by removing many background spectrum components that have nothing to do with scattered light reflections. Before data modeling, the MSC technique will also eliminate scatter effects from the data matrix [18].

The Savitzky-Golay derivative pre-processing technique is also used in this study (9-point smoothing window, first-order polynomial, SG-1stD). The Savitzky-Golay derivative method uses a filtering technique that flattens the signal while lowering signal components at low frequencies through differentiation to reduce interference in the high-frequency spectrum. As a result, critical spectral features become more evident [19]. The selection of 9-point windows and first-order polynomials is a method for retaining essential features of the data. A small window is ineffective enough in reducing noise, while a too-large window can remove crucial information from the data. Choosing a first-order polynomial that is too high is aggressive in smoothing the data, potentially removing significant information.

A combined MSC and SG-1stD pre-processing approach is also used. The original and pre-processed spectra in the entire spectral range are used to construct the PLS regression model. Data-centering processes are still carried out before PLS modeling despite using different pretreatment techniques. Unscrambler X 10.3 software (CAMO Inc., Oslo, Norway) was used for all data pre-processing and chemometric calculations.

2.5 Procedural steps and parameters used in the data processing and modeling

The procedural stages in data processing and modeling begin with detecting outliers in all samples in spectral data (represented by 1554 variables), followed by removing samples or spectra that are considered outliers from the data set. The next stage is to divide the data group into calibration and validation data sets. Then, the model was developed using the PLS method using calibration and reference data collection. In developing this model, the maximum number of PCs used is 15; however, the optimal number of PCs is determined based on the number of PCs that provide a slight difference in variance between the calibration data set and the internal validation data set. Apart from the original model, a model with some data pre-processing was also developed. Finally, the resulting models were tested using external validation data (i.e., sample not used for model development), and their performance was analyzed to determine the best model for predicting the water content of Sumatran roasted coffee beans.

2.6 Identify outliers and sample set design

Identifying outliers is crucial before creating a multivariate calibration. The stages used in this study's outlier identification process are based on [20]. Principal component analysis (PCA) is used as the initial step to select and eliminate spectra that are thought to be outliers that could otherwise obstruct model construction. For each Y variable, the second stage involves finding aberrant samples by combining residual F and Hotelling's T-squared statistics (T^2). Samples with F and T^2 statistic values above the 95% (i.e., significance level) threshold are outliers. Outlier samples are then eliminated. The Kennard-Stone algorithm is used in the fourth phase to divide the remaining components into the calibration and validation sets, with a 2:1 ratio. The validation set is used to evaluate the produced model after it has been developed using the calibration set.

2.7 Partial least squares (PLS) regression

The calibration model is created by connecting the NIR spectrum with the measurement reference using the PLSR technique, where the NIR spectrum is viewed as a matrix. The calibration model is created by connecting the NIR spectrum with the measurement reference using the PLSR technique, where the NIR spectrum is viewed as a matrix. When doing internal cross-validation, the calibration model is constructed using the calibration dataset and validated using the K-fold cross-validation method, which is applied randomly with ten segments containing five samples. The minimum value of the root mean square error of cross-validation (RMSECV) is used to calculate the appropriate number of factors (LV). We also undertake further validation using an external dataset as a kind of external validation to verify the performance of the calibration model that has been constructed. Several parameters are used to evaluate the calibration model, including the root mean squared error of calibration (RMSEC), the root mean squared error of prediction (RMSEP), the coefficient of determination for calibration (Rc^2), the coefficient of determination for cross-validation (Rcv^2), the coefficient of determination for prediction (Rp^2), and the residual performance deviation (RPD). The relationship between a reference value's standard deviation (SD) and RMSEP is described by the statistic known as RPD. RPD values can distinguish between high and low levels between 1.5 and 2.0 and demonstrate that quantitative estimations are possible between 2.0 and 2.5. The prediction is considered good or extremely good if the value exceeds 2.5 or 3.0 [21]. If the RPD is high, meaning the RMSEP is smaller than the SD, a calibration model is said to be reliable and accurate.

3. RESULTS AND DISCUSSION

3.1 NIR spectral features

The original NIR spectrum of Sumatran roasted coffee beans is shown in Figure 1. The original NIR spectrum in the 1000-2500 nm range is broad and overlaps several spectral peaks. The peak of the NIR absorption spectrum of Sumatran roasted coffee beans appears at a wavelength of around 1215 nm, which indicates the presence of caffeine [22], which occurs due to C-H str., the second overtone of the CH_2 structure. Another absorption peak located at a wavelength of 1450 nm occurs due to O-H str. The first overtone of the starch structure, H_2O, occurs at a wavelength of 1935 nm (close to 1940 nm) due to O-H str. and O-H def. from the structure of H_2O [23].

The high absorption at wavelengths of 1450 nm and 1940 nm indicates the presence of water content associated with O-H bonds in hydroxyl groups in harmonic and combination forms [24]. It was further explained [25] that in foodstuffs that have a water content of around 70-90%, there are visible absorption bands at wavelengths almost the same as the absorption bands of pure water, namely in the range from 1400 to 1410nm. In contrast, the absorption band associated with free water was detected at around 1430 nm in dry foodstuffs. What is clear is that roasted coffee beans, a food with low water content, show high absorption at a wavelength of 1450 nm.

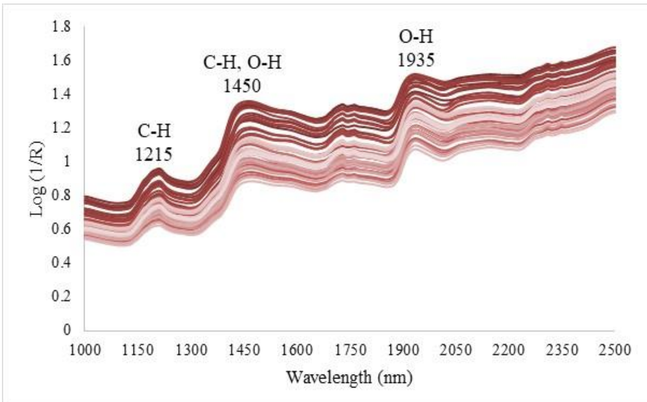

Figure 1. Spectral features of a typical absorption spectrum of Sumatran roasted coffee beans at a wavelength of 1000-2500 nm

3.2 Sample outliers' elimination

One outlier spectrum was found in all original spectra's initial PCA score plots, namely spectrum number 4 (Figure 2) because the statistical significance level of F and T^2 exceeds the 95% threshold. Next, a PLS model of the water content of Sumatran roasted coffee beans was built from 53 original spectra. Based on the F-residual plot and Hotelling T-squared statistics (T^2), which were used to find outliers for each Y variable.

Figure 3 shows that no outlier samples were found because none of the samples were outside the rectangle. Thus, in building the model, the 53 samples were divided into two sets, namely the calibration set (2/3 sample = 35), applied to develop the model, and the prediction set (1/3 sample = 18), which was used to assess the robustness of the developed model. Table 1 shows the mean, range, standard deviation of water content, and median values in the calibration and validation data sets. The highest and lowest values belong to the calibration set, so the data in the validation set can be used to prove and assess the calibration model. This is because the calibration model will provide accurate results in predicting concentrations if tested on similar samples.

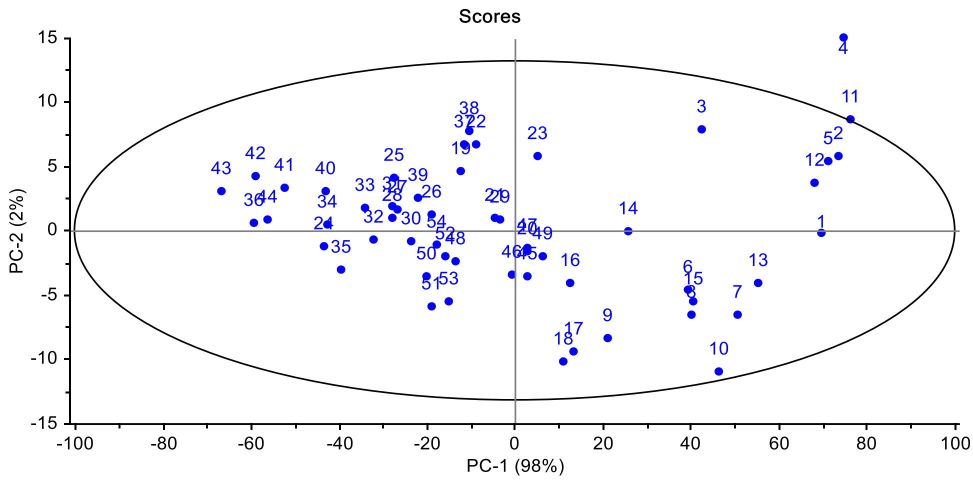

Figure 2. Projection of the PCA and Hotelling T^2 ellipse methods for outlier data detection

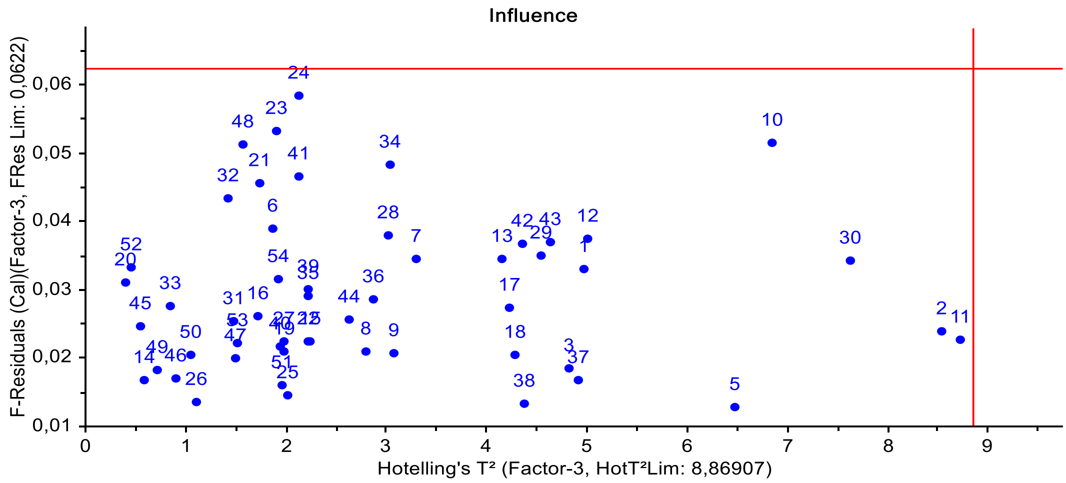

Figure 3. F-residual plot and Hotelling T-squared statistics (T^2) for outlier detection for each Y variable

Table 1. Descriptive statistics of water content in the calibration and validation dataset

Parameter	Set Calibration	Set Validation
Mean (%)	0.213	0.207
Range (min-max) (%)	0.160 - 0.302	0.161 - 0.298
Std Deviation (%)	0.039	0.037
Median	0.207	0.207

3.3 Building PLS regression models

The PLS regression model was built using wavelengths of 1000–2500 nm as the independent variable (totaling 1554 variables), and data on the water content of Sumatera roasted coffee beans as the dependent variable (totaling 53 variables). The PLS regression model uses dimensionality reduction and simultaneously looks for the best linear relationship between the independent and dependent variables. Dimensionality reduction produces latent variables (LVs) whose numbers can be selected to avoid overfitting and optimize model performance.

In this research, the optimal number of latent variables varied from 3 to 6 (Table 2). Also, MSC, SG9-1stD, and the combination of MSC and SG9-1stD pre-processing were used to improve the quality of the NIR spectrum data used to predict the water content of Sumatran roasted coffee. When building a model, dividing the data into training and testing sets is necessary to prevent overfitting. The training set data is used to train the model, and the test set is used to test the model's reliability. This research has two test sets: internal validation using the cross-validation method and external validation using independent data (data not used during the training process or processes that have not been previously validated).

Table 2 presents the findings concerning the calibration model for Sumatran roasted coffee beans. Based on the values of Rc^2, Rcv^2, and Rp^2, all calibration models show excellent models because they have R^2 values above 0.91 [21]. Furthermore, the resulting models offer low RMSEP values, ranging from 0.003-0.006 (%), which indicates that the calibration models can predict the water content of Sumatran roasted coffee beans with a high level of accuracy. Calibration models with more robust prediction performance are characterized by higher Rc^2, Rcv^2, and Rp^2, and lower values of RMSEC, RMSECV, and RMSEP [26]. This study's RPD values ranged from 5.974 to 12.216, indicating an excellent model. The water content of Sumatran roasted coffee beans is visualized in Figure 4(a-d) after being measured using the reference method and predicted using the PLSR approach.

Table 2. The performance of the calibration model for Sumatran roasted coffee beans

Pre-Processing Method	LVs	Calibration		Cross-Validation		Prediction		
		Rc^2	RMSEC (%)	RMSECV (%)	Rcv^2	Rp^2	RMSEP (%)	RPD
Raw Data	4	0.980	0.006	0.007	0.972	0.987	0.005	7.570
MSC	3	0.984	0.005	0.006	0.980	0.981	0.005	7.222
SG9-1stD	6	0.991	0.004	0.005	0.982	0.981	0.006	5.974
MSC + SG9-1stD	4	0.992	0.003	0.004	0.990	0.995	0.003	12.216

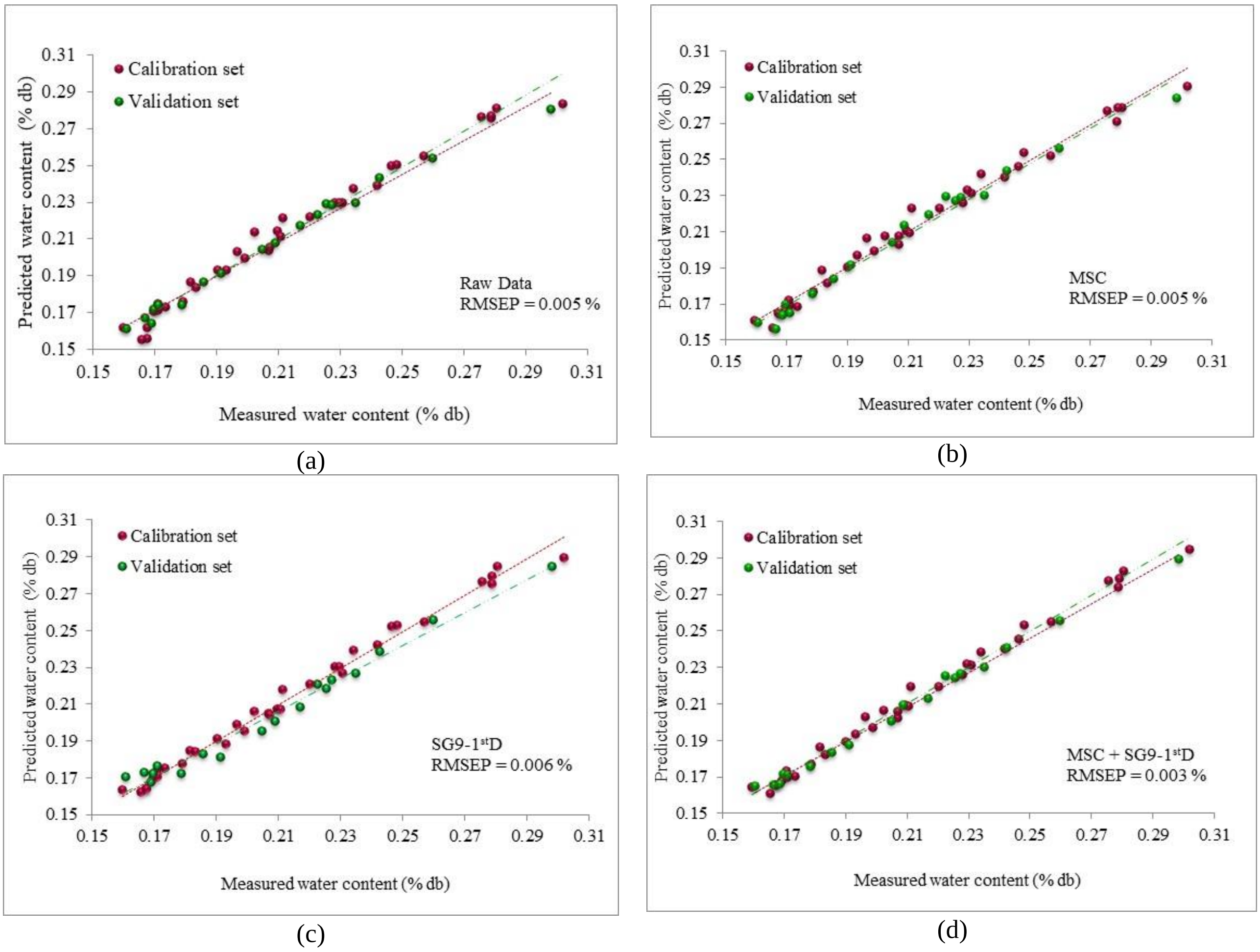

Figure 4. The comparison between measured and predicted water content for calibration and validation datasets, each subjected to different pre-processing methods

The parameters RMSEC, RMSECV, RMSEP, Rc^2, Rcv^2, Rp^2, and RPD show that using raw data produces a model with good performance. Compared with raw data, the approach with the MSC pre-processing method improves the model performance in various low-level parameters, such as RMSEC and RMSECV. Other values remain high, indicating the existence of a strong model. The model's performance is improved by comparing the SG9-1stD pre-processing approach with the raw data. Lower RMSEC and RMSECV values indicate better estimation precision. However, the RPD value obtained with the SG9-1stD pre-processing method is slightly lower than the MSC pre-processing approach. The calibration model works well with the MSC+ SG9-1stD pre-processing method. When compared with previous preprocessing techniques, values such as RMSEC = 0.003%, RMSECV = 0.004%, RMSEP = 0.003%, Rc^2 = 0.992, Rcv^2 = 0.990, Rp^2 = 0.995, and RPD = 12.216 show significant improvements. These performance parameters show that combining these two pre-processing approaches produces the most accurate prediction of the moisture content of Sumatran roasted coffee beans.

In our study, the R^2 values represent the coefficient of determination which measures how well the predicted values from our models match the actual values. The metrics Rc^2, Rcv^2, and Rp^2 specifically denote the coefficient of determination for calibration, cross-validation, and prediction, respectively. A high Rc^2 value indicates a strong correlation between the observed and predicted values in the calibration dataset.

In the context of our study, the Rc^2 value of 0.99 suggests that 99% of the variance in the observed data can be explained by our model, underscoring its accuracy in the calibration phase. Similarly, the Rcv^2 value measures the model's predictive power during cross-validation. A Rcv^2 value close to Rc^2, as observed in our study ($Rcv^2 = 0.98$), indicates that the model performs consistently even with unseen data, highlighting its robustness. The Rp^2 value represents the model's predictive accuracy on an independent dataset. Our Rp^2 value of 0.97 demonstrates that the model retains its high level of accuracy, explaining 97% of the variation in the prediction set, reinforcing the model's applicability in real time NIRS applications.

Choosing the appropriate pre-processing method involves balancing the need for noise and artifact reduction with the preservation of relevant spectral data. The selection depends on the nature of the dataset and the specific requirements of the modeling task. Our findings suggest that while a combination of MSC and SG is superior for our particular dataset and objectives, one must consider the specific characteristics and requirements of their analysis when selecting a pre-processing method.

4. CONCLUSIONS

This presented study set out with the objective to evaluate the effectiveness of NIR spectroscopy as a non-invasive approach for predicting the water content in roasted Sumatran coffee beans, aiming to enhance quality control measures within the coffee industry. By employing a combination of multiplicative scatter correction (MSC) and Savitzky-Golay (SG9-1stD) pre-processing techniques, we have successfully developed an accurate prediction model that meets and exceeds our initial objectives. The application of NIR spectroscopy, as demonstrated in our research, directly contributes to the improvement of quality assessment practices, aligning with our goal to provide a reliable, efficient solution for maintaining the quality and competitiveness of roasted coffee beans on a global scale.

To ensure the universal applicability of our model across all coffee varieties and processing conditions, further validation studies are recommended. Practically, the implementation of NIR spectroscopy in the coffee industry, as suggested by our research, could revolutionize standard quality control processes. We recommend that coffee producers and quality assurance teams incorporate NIR spectroscopy techniques, specifically using the MSC and SG9-1stD pre-processing methods, into their routine assessment routines to ensure the highest quality of roasted beans.

Despite the promising applications of NIR spectroscopy in quality control, the implementation process within the industry is not without its challenges. Accessibility to the necessary equipment and the level of expertise required might vary significantly across different regions and scales of coffee production. Therefore, an assessment of the economic and logistical feasibility of adopting NIR spectroscopy should precede its implementation.

Additionally, exploring the integration of this technology with other quality assessment parameters could provide a more comprehensive toolkit for the coffee industry. Unresolved questions regarding the scalability of this technology and its optimization for diverse coffee processing environments remain, highlighting areas for future work.

In brief, this research underscores NIR spectroscopy's potential to significantly advance quality control practices in the coffee industry. By establishing a robust model for the non-invasive prediction of water content in roasted Sumatran coffee beans, it not only enriches the domain of coffee quality assessment but also sets the stage for further innovations in the field.

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