QUALITY EVALUATION OF THE PALM MESOCARP USING NEAR-INFRARED SPECTROSCOPY AND CHEMOMETRICS METHODS

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ABSTRACT

Palm oil, a globally significant vegetable oil, has diverse applications due to its unique fatty acid profile. Its quality is influenced by factors such as fruit maturity and oil content. This study investigates the feasibility of near-infrared spectroscopy (NIR) as a rapid, non-destructive method for predicting key palm oil quality parameters. Traditional reference methods measured oil content, moisture, acidity, DOBI, and fatty acid composition in palm mesocarp sliced (PMS) and palm mesocarp dried (PMD) samples. NIR spectra were collected and analyzed using chemometric techniques to develop calibration models. Results demonstrated the potential of NIR for accurately predicting oil content, acidity, and specific fatty acids in PMD samples. While predictive performance for stearic acid was slightly lower, it remained suitable for screening. For PMS, the best results were obtained from moisture and DOBI. The acidity model in PMS underperformed, possibly due to the limited number of samples used for calibration. Regarding the carotene model, there is a potential margin for enhancing its accuracy. These findings highlight the value of NIR as a time-efficient and environmentally friendly alternative to traditional analytical methods, offering significant benefits to the palm oil industry.

Palavras-chave: Palm oil; Multivariate calibration; Palm fruits; Partial least square; Non-destructive analysis.

INTRODUCTION

Palm oil (*Elaeis guineensis* Jacq.) is a globally significant oil crop, with palm oil being widely used in various edible and non-edible products. This surge is driven by increasing global demand due to population growth and rising living standards. The *Elaeis* genus comprises *E.*

guineensis, the dominant species in commercial plantations, and *E. oleifera*. Breeding programs are developing inter-specific hybrids between these species to address fatal yellowish and improve oil quality. These hybrids offer a diverse fatty acid profile with lower acidity, higher unsaturated fatty acids, sterols, and vitamins, making them more suitable for various industrial applications, (España et al., 2018). To address these issues and ensure quality, researchers are exploring innovative methods.

Near-infrared (NIR) spectroscopy is a promising solution for rapid and non-destructive palm oil quality parameters analysis. This technique utilizes light absorption in the near-infrared region to obtain information about the chemical composition of the biomass (Cozzolino, 2022). In the palm oil industry, NIR spectroscopy is a game-changer. It can rapidly assess oil content, a critical parameter for monitoring the productivity of palm poç trees content (Gürbüz et al., 2023). Additionally, NIR spectroscopy has been successfully applied to analyze various quality parameters of palm oil, including acidity, moisture, and fatty acid composition (Sudarno et al., 2017; Li et al., 2020). NIR spectroscopy has the potential to revolutionize the palm oil industry by providing rapid, non-destructive, and accurate analysis of various quality parameters. By adopting this technology, stakeholders can improve the quality and sustainability of palm oil production, ensuring a more reliable and valuable product for consumers. This study aimed to develop a rapid method for determining acidity, oil and moisture content, fatty acids profiles (palmitic, stearic, oleic, and linoleic acids), DOBI, and carotenes through NIR spectroscopy calibration and chemometrics methods, testing to ways of the capture of spectrums in dried-ground palm mesocarp and inf fresh mesocarp slices.

METHODOLOGY

Palm mesocarp samples from various planting materials and maturity levels of *E. guineensis*, *E. oleifera*, and interspecific hybrids were collected in Brazil from 2020-2023. Traditional bunch analysis was followed, with samples divided into sliced mesocarp (PMS) and dried mesocarp (PMD). NIR spectroscopy analyses were conducted on 234 PMS and 392 PMD samples. Chemical analysis was performed to extract oil from dry pulp fruits according to Am 5-04 (AOCS, 2005). The acid content was measured using the AOCS Method Cd 3d-63 (AOCS, 2005). The moisture determination was performed according to Sluiter and Sluiter, 2010). The

fatty acids profile was determined according to the procedure reported by the AOCS Methods Ce 1-62 and Ce 2-66 (AOCS, 2005). DOBI is the numerical ratio of spectrometric absorbance at 446 nm to 269 nm; it was determined following ISO 17932 (Ribeiro et al., 2018). Total carotenes were determined by spectrophotometry using an adapted protocol derived from the method described by (Porim, 1990; Rossi et al., 2001). NIR spectra were recorded in reflectance mode using a NIRFlex 500 spectrometer (Buchi Labortechnik, Flawil, Switzerland). The PMD and PMS samples were loaded into a Petri dish of 9 cm inner diameter, and the NIR spectrum was obtained at a room temperature of 25 ± 2 °C. for the wavelength range between 1,000 and 2,500 nm. NIR spectral data were pretreated and analyzed using Unscrambler 10.5 software. Standard normal variance (SNV) and Savitzky–Golay first derivative were applied for scattering correction and baseline shifts. Partial Least Squares (PLS) were used for constituent quantification, with the number of latent variables determined based on RMSECV to avoid overfitting. The best calibration model was evaluated based on R^2c, RMSEC, R^2p, and RMSEP. The Range Error Ratio (RER) was used to assess model goodness, with RER ≥10 indicating acceptable quality control. The SD to RMSEP (RPDp) ratio was used to evaluate predictive power, with RPDp < 2.5 indicating insufficient predictive power, 2.5-3 indicating good predictive ability, and >3 indicating excellent predictive performance. A t-test was used to confirm significant differences between reference and predicted values (p<0.05).

RESULTS AND DISCUSSION

Table 1 shows the effectiveness of NIR spectroscopy coupled with PLS regression for estimating the constituents of palm mesocarp. The PLS models achieved good accuracy (R^2p > 0.85) for predicting both Oil_{fb} and Oil_{db} content in both PMD with RER > 11, but Oil_{db} PMS did not perform as well as PMD samples. The best calibration model was Oil_{db} (PMD) with R^2_c and R^2_p 0.91, RMSEP 3.03, RER 14.9, and RPD_p 3.5. This aligns with previous research by Sudarno et al. (2017), who successfully used NIR-PLS models for oil content prediction in palm mesocarp and obtained an R_{2c} of 0.996 and SEP of 1.42 for homogeneous samples but with high latent variables (15). The moisture calibration model showed better results for PMS than PMD samples (Table 1), which could probably be attributed to the relatively narrow moisture range in dried samples compared to the broader range used for PMS calibration. The PMS

calibration models had better RER 10 and RPD_p 2.8 results than the PMD calibration models. The oil and moisture contents in the mesocarp are two parameters used as a reference to determine the ripeness grade of palm oil fresh fruit (Silalahi et al., 2016). The acidity model in PMD (Table 1) displayed excellent prediction accuracy ($R^2p = 0.95$), highlighting its potential for monitoring free fatty acid content in the range of 2 to 22.3 mg KOH. g^{-1}, a crucial quality parameter. However, the PMS model underperformed, possibly due to the limited number of samples used for calibration. The palmitic, stearic, oleic, and linoleic acid models (Table 1) generally yielded promising results ($R^2p > 0.84$). Low RMSEP was obtained for calibration models using a PMD sample set. The RER was >10 for palmitic, oleic, and linoleic acids (in the PMD sample set), indicating that excellent models were obtained at the level of quality control. For stearic acid, the RER was 7.1 (in the PMD sample set), and all the other models for the PMS sample set obtained RER <10 and qualified for screening calibration. This aligns with research by Hussain et al. (2023), who demonstrated the potential of NIR for palm oil fatty acid determination.

Table 1 – Calibration and validation results for estimating the chemical properties of palm oil mesocarp from NIR reflectance spectra using Partial Least Square regression

Constituent		Cal set	R^2_c	RMSEC	R^2_{CV}	RMSECV	Val set	R^2_p	RMSEP	RER	RPD_p	*p-value*
Oil_{fb}	**PMD**	237	0.91	3.34	0.89	3.76	118	0.90	3.39	13.8	3	0.79
	PMS	138	0.86	4.35	0.86	4.70	73	0.85	4.51	11	2.6	0.29
Oil_{db}	**PMD**	219	0.91	3.17	0.91	3.27	109	0,91	3.03	14.9	3.5	0.42
	PMS	151	0.85	4.41	0.84	4.70	72	0.76	5.72	9	2	0.36
Moisture	**PMD**	176	0.83	0.56	0.79	0.63	87	0.73	0.68	8.8	2.5	0.33
	PMS	142	0.91	3.43	0.91	3.57	65	0.87	4.05	10	2.8	0.60
Acidity	**PMD**	88	0.93	1.67	0.88	2.16	27	0.95	1.30	16.3	5.0	0.31
	PMS	29	0.89	2.62	0.59	4.44	9	0.78	2.94	5.7	2.1	0.49
Palmitic Acid	**PMD**	262	0.94	2.09	0.93	2.27	130	0.94	2.05	14.1	4.1	0.62
	PMS	149	0.91	2.61	0.90	2.75	76	0.86	3.22	9.1	2.7	0.22
Stearic acid	**PMD**	232	0.75	0.62	0.71	0.66	119	0.66	0.69	7.1	1.7	0.19
	PMS	127	0.80	0.48	0.76	0.54	71	0.62	0.69	6.2	1.6	0.99

Oleic Acid	**PMD**	254	0.95	1.92	0.95	1.92	128	0.92	2.49	12.3	3.5	0.87
	PMS	146	0.88	3.05	0.87	3.28	72	0.84	3.37	8.9	2.5	0.43
Linoleic Acid	**PMD**	245	0.87	0.61	0.84	0.67	121	0.86	0.60	16.2	2.7	1.0
	PMS	135	0.59	1.18	0.57	1.23	72	0.49	1.29	6.6	1.4	0.44
DOBI	**PMD**	244	0.77	0.46	0.49	0.73	121	0.73	0.50	9	1.9	0.27
	PMS	128	0.84	0.34	0.40	0.86	60	0.86	0.41	10	3	0.67
Carotenes	**PMD**	218	0.84	307.84	0.78	369.92	118	0.82	330.02	8.7	2.4	0.74
	PMS	140	0.89	351.88	0.86	400.80	72	0.86	410.98	11.2	2.4	0.91

PMD: Palm mesocarp dried; PMS: Palm mesocarp slice; Oil_{fb}: Oil fresh base, Oil_{db}: Oil dry base, Moisture, palmitic acid, stearic acid, oleic acid, linoleic acid, and carotenes results expressed in %. DOBI: deterioration of bleachability index; PMD: Palm mesocarp dried, PMS: Palm mesocarp slice

NIR spectroscopy effectively predicts DOBI in palm mesocarp, with high R^2 and low RMSEP values. This study shows that determining DOBI in PMS is the most effective approach since no literature reports directly using near-infrared spectroscopy to assess DOBI in palm mesocarp. This study also shows promising results for carotene prediction with the PMD sample set. The model achieved a high coefficient of determination (R^2c) of 0.86, indicating a good fit between predicted and actual carotene values.

FINAL CONSIDERATIONS

The study reports that applying NIR spectroscopy and chemometrics methods to determine the oil content, moisture, acidity, palmitic, stearic, oleic, and linoleic acids, DOBI, and carotenes in slice or dry and ground mesocarp was successfully achieved with good precision and the results do not show differences from reference methodologies.

This methodology showed that the NIR spectroscopy technique for different constituents from palm mesocarp would be most beneficial as it is simple, rapid, and low-cost. Additionally, it is friendlier to the environment due to avoiding chemical reagents, which significantly benefits the palm oil industry.

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