

MONITORING OXIDATIVE LEVELS OF FRYING OILS USING FTIR SPECTROSCOPY AND MULTIVARIATE CALIBRATION

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ABSTRACT

Objective: To develop a rapid reliable technique based on Fourier transform infrared-attenuated total reflectance (FTIR-ATR) spectroscopy in combination with multivariate calibrations for prediction of frying oil quality, namely acid value (AV), iodine value (IV) and peroxide value (PV).

Methods: FTIR spectra were directly obtained and subjected to optimization and spectral treatments including a selection of wavenumbers region and spectral derivatization. The condition selected was based on its capability to provide the highest coefficient of determination (R^2) and the lowest root mean square error of calibration (RMSEC) and root mean square error of prediction (RMSEP) for the relationship between actual values of AV, IV, and PV as determined using standard titrimetric methods and predicted values as determined by FTIR spectroscopy aided with multivariate calibrations.

Results: Using optimized condition, FTIR spectroscopy combined with multivariate calibrations could be successfully used for prediction of AV, and PV. Acid value (AV) could be determined using the first derivative spectra at wavenumbers of 1524-658 cm^{-1} . The R^2 of 0.973 (in calibration model) and 0.932 (in prediction model) with low RMSEC and RMSEP values was obtained. Iodine value (IV) was best predicted using principle component regression (PCR) with normal FTIR spectra at the combined wavenumbers region of 3076-2783 and 1811-656 cm^{-1} . PCR using normal spectra at combined wavenumbers region of 3076-2783 and 1811-656 cm^{-1} was also selected for prediction of PV.

Conclusion: FTIR spectroscopy in combination with multivariate calibration has been successfully used for prediction of acid value, iodine value and peroxide value in frying oils. The developed method could be an alternative technique for analysis of these values to perform quality assurance of frying oils.

Keywords: FTIR spectroscopy, Oil quality, Multivariate calibration, Attenuated total reflectance

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INTRODUCTION

The quality of frying oil (FO) closely affected fried foods [1]. During frying, oil has been subjected to be heating at high temperatures at prolonged periods with the presence of water and air, which lead to some complex chemical reactions including thermal degradation, hydrolysis, polymerization, and oxidation [2, 3]. The chemical compounds resulted from these reactions are not only producing undesirable components but also affecting the quality of food flavor [4]. As a consequence, the quality control of FO using rapid and reliable methods should be developed. Several parameters have been used for evaluation of FO including acid value (AV) or free fatty acids (FFA), peroxide value (PV), iodine value (IV) and total polar compounds (TPC) [5, 6], and its authenticity [7, 8].

The standard analytical methods used for monitoring the quality of fats and oils as appeared in Association of Official Analytical Chemists (AOAC) and International Standardization Organization (ISO) are based on wet chemical methods such as titrimetric which involved some solvents and reagents and in some cases using sophisticated instruments such as gas chromatographic which are expensive, require lengthy sample preparation, and, in some cases, depend on advanced instruments and skillful analyst [9, 10]. Thus, some simple methods based on spectroscopic methods could be developed as an alternative method to overcome the drawbacks of wet chemical methods and the complexity of sophisticated instruments. The results of FTIR spectroscopy have been reported to correlate with those using wet chemical methods [11, 12].

Due to its property as fingerprint analytical techniques [13], FTIR spectroscopy in combination with chemometrics have been developed for analysis of acid value [14, 15], the peroxide value of FO [16], iodine value [17], and anisidine value [18]. However, these oil parameters were determined individually, and there are limited reports regarding the determination of acid value (AV), peroxide value (PO) and iodine value (IV) simultaneously. Therefore, this research was aimed to determine

AV, PO and IV simultaneously using FTIR spectroscopy in combination with multivariate calibrations of principle component regression (PCR) and partial least square regression (PLSR).

MATERIALS AND METHODS

Materials

Frying oils and used frying oils were obtained from Samarinda, East Kalimantan, Indonesia. The other reagents and solvents used were of pre-analytical grade obtained from E. Merck (Darmstadt, Germany).

Determination of acid value

Acid value (AV) of FO samples was determined using titration method as appeared in the standard method of the American Oil Chemists' (AOCS). A-10.0 g of FO samples were accurately weighed and dissolved in 100 ml ethanol-ethyl ether mixture (1:1 v/v). This solution was then titrated using standardized KOH-ethanolic solution using phenolphthalein as indicator until the pink-violet color was observed. AV was expressed as the number of mg KOH needed to neutralize free fatty acids in 1 g of FO samples. AV was calculated as:

$$AV = \frac{\text{Volume KOH}}{\text{g sample}} \times N_{\text{KOH}} \times 56.1$$

Determination of iodine value

Iodine value (IV) was determined according to AOCS titration method. A-1.0 g of FO samples was added with 20 ml cyclohexane-acetic acid mixture (1:1 v/v). The solution was added with 25 ml of Wijs solution (iodine monochloride, ICl) and was kept in the dark condition for 1 h. The mixture was added with 20 ml saturated KI solution and 150 ml distilled water, shaken homogeneously, and titrated with 0.1 N sodium thiosulphate 0.1 N using 1 mL of starch indicator 0.05% until the color became clear. The blank titration was also carried under the similar condition without the addition of FO samples. IV was calculated as:

$$IV = \frac{(V_b - V_s)}{\text{g sample}} \times N_{\text{thio}} \times 12.69$$

V_b is volume (in ml) of thiosulphate used for blank titration and V_s is volume (in ml) of thiosulphate used for sample titration.

Determination of peroxide value

Determination of peroxide value (PV) was performed using the titrimetric method according to ISO (3960:2001) as in Liang *et al.* (2013). An approximately of 5.0 g of FO samples were placed into iodine flask and was dissolved in the solution mixture of 150 glacial acetic-acid isooctane (3: 2, v/v). The solution was added with 0.5 mL saturated solution of KI. The mixture was then shaken vigorously for 0.5 min and allowed in the dark condition for another 3 min. The solution was added with 30 mL distilled water and was titrated using sodium thiosulphate 0.01 N using 1 mL of starch indicator 0.05%. Titration was stopped if blue colour of solution just disappeared. The blank titration was also carried out under the similar condition without the addition of FO samples. PV was calculated as:

$$PV = \frac{(V_s - V_b)}{\text{g sample}} \times N_{\text{thio}} \times 1000$$

Where PV is peroxide value (in meq/kg), V_s is volume (in ml) of thiosulphate used for sample titration, V_b is volume (in ml) of thiosulphate used for blank titration, N_{thio} is normality of thiosulphate.

Measurement of FTIR spectra

FTIR spectra of FO samples were scanned using FTIR spectrophotometer (Nicolet 6700 from Thermo Nicolet Corp., Madison, WI) equipped with a detector of deuterated triglycine sulphate (DTGS) and KBr as a beam splitter. FTIR

spectrophotometer was connected to computer operating systems using software OMNIC operating system Version 7.0 from Thermo Nicolet (Madison, WI, USA). The sampling technique used was Attenuated Total Reflectance kit (ATR, Smart ARK, Thermo Electron Corp.) using ZnSe crystal. FTIR spectra were read at the mid-infrared region, 4000–650 cm^{-1} , using absorbance mode to facilitate the quantitative analysis based on Lambert-Beer law.

Chemometrics analysis

The chemometric analyses were carried out using TQ Analyst software included in the FTIR instrument. Prediction of AV, IV, and PV was facilitated with multivariate calibration of partial least square regression (PLSR) and principal component regression (PCR) [19, 20]. PLSR algorithm is an effective multivariate calibration which takes the advantages of multiple linear regression and PCR. PLSR has a relatively simple model with strong predictive capability, making it suitable for FTIR spectral treatment [21, 22].

RESULTS AND DISCUSSION

In this study, the quality of frying oils was evaluated by determining several parameters namely acid value (AV), peroxide value (PV), and iodine value (IV) simultaneously using FTIR spectroscopy in combination with multivariate calibrations of PLSR and PCR. Acid value (AV), used for evaluation of fatty acids released, can be taken into account as the precursors of lipid oxidation products in which the higher AV, the lower quality of oils [23].

Iodine value (IV) is used to measure the unsaturation degree of double bonds in oils so that the decrease of IV indicated a decrease in double bonds, and it indicated oxidation of oils [24, 25]. Peroxide value (PV) could be used as an indicative of oxidation of oils in the initial stages of oxidation [1]. Table 1 indicated of AV, IV, and PV of frying oils.

Table 1: Acid value (mg KOH/g oil), peroxide value (meq/kg) and Iodine value (gI₂/100 g) of frying oils

Samples	Acid value (mg KOH/g oil)	Peroxide value (meq/kg)	Iodine value (gI ₂ /100 g)
KM	0.1988	2.8789	40.4920
K2B	0.2651	2.9908	38.5182
A1	1.5244	12.8550	11.1092
A2	1.0605	11.6302	17.1950
A3	0.6628	5.7692	26.7554
L1	1.9884	18.3053	2.0627
L2	0.5302	4.0625	30.6298
L3	0.7291	5.9451	24.1855
G1	0.5965	4.9745	28.0312
G2	0.7954	6.7978	22.8058
G3	0.3977	3.8922	33.8224

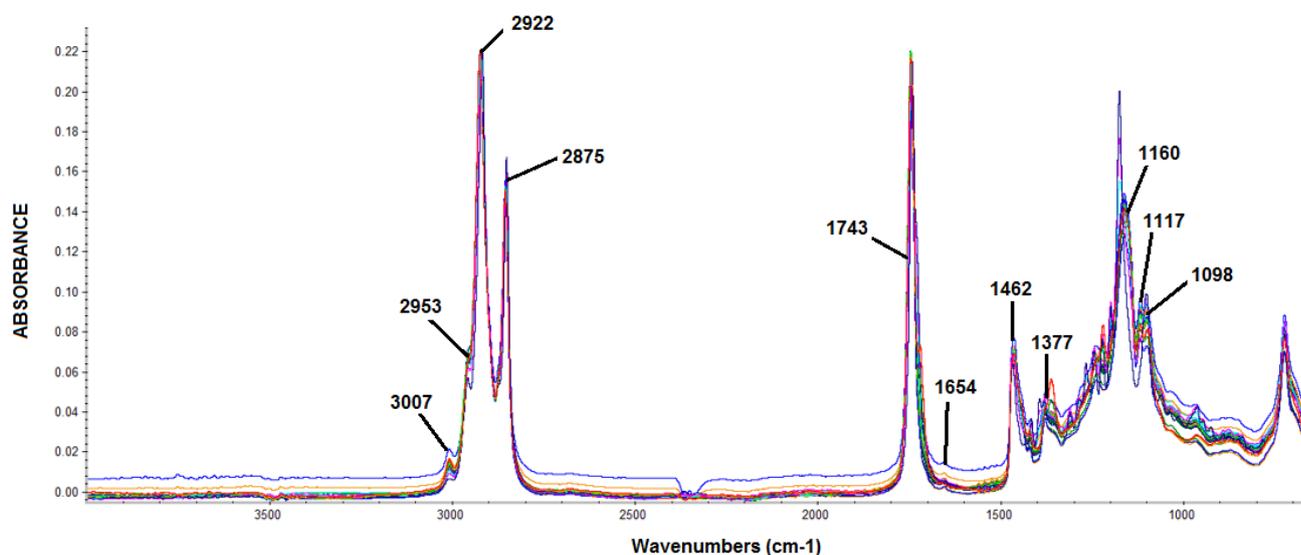


Fig. 1: FTIR spectra of frying oils (palm oils), scanned at mid-infrared region (4000-650 cm^{-1}) using attenuated total reflectance

The standard methods for analysis of AV, IV and PV were titrimetric methods which were laborious and involving chemical reagents, therefore, in this study, FTIR spectroscopy in combination with multivariate calibrations (PLSR and PCR) was developed for prediction these values with the main advantage of simplicity, ease in analysis, and allowing simultaneous analysis. Fig. 1 revealed FTIR spectra of frying oils scanned at mid-infrared regions which exhibited characteristics peaks and shoulders present in triglycerides. Each peak and shoulders indicated the functional groups responsible for IR absorption. The identification of functional groups in each wavenumber can be found in [6, 7, 12]. Peaks at 3007 cm^{-1} were due to cis =CH-stretching vibration, peaks at 2953 and 2922 were corresponding to the asymmetric stretching vibration of-

CH_3 dan- CH_2 -, respectively. The presence of carbonyl groups was confirmed by a peak at 1743 cm^{-1} . Peak at 1654 cm^{-1} was due to stretching vibration of C=C. The presence of -CH_2 and CH_3 was also confirmed by bending vibrations at 1462 and 1377 cm^{-1} , respectively. In addition, the peaks at 1160, 1117 and 1098 cm^{-1} were due to C-O stretching vibration.

Table 2 compiled the performance of FTIR spectroscopy and multivariate calibrations for prediction of acid value (AV). Several wavenumbers and also spectral treatments (normal, first derivative, and second derivative) were also optimized to obtain the best condition for such prediction. The spectral derivative is applied to get the best resolution among overlapping peaks, but spectral derivatization could make lower sensitivity than normal spectra.

Table 2: The optimization of FTIR spectra in combination with multivariate calibration for the prediction of acid value

Multivariate calibrations	Wavenumber (cm^{-1})	Spectra	Calibration		Validation	
			R ²	RMSEC	R ²	RMSEP
PCR	3040-658	normal	0.922	0.201	0.987	0.153
		der-1	0.7035	0.368	0.7231	0.415
		der-2	0.8205	0.296	0.6699	0.422
	1825-658	normal	0.7627	0.335	0.9246	0.278
		der-1	0.7622	0.335	0.628	0.475
		der-2	0.937	0.181	0.8824	0.274
	1524-658	normal	0.9172	0.206	0.896	0.372
		der-1	0.9726	0.121	0.9318	0.253
		der-2	0.9689	0.128	0.9387	0.239
	3040-2784and 1825-658	normal	0.9338	0.185	0.9775	0.264
		der-1	0.7034	0.368	0.7155	0.421
		der-2	0.9399	0.177	0.7805	0.353
	3040-1664and 1524-658	normal	0.9201	0.203	0.9876	0.149
		der-1	0.7027	0.369	0.7182	0.417
		der-2	0.8075	0.306	0.6552	0.43
	3040-2784and 15244-658	normal	0.931	0.189	0.972	0.253
		der-1	0.7134	0.363	0.7604	0.382
		der-2	0.9126	0.212	0.7385	0.381
	3040-2784, 1825-1664and 1524-658	normal	0.9277	0.193	0.9729	0.26
		der-1	0.703	0.369	0.7057	0.426
		der-2	0.8923	0.234	0.6657	0.427
PLSR	3040-658	normal	0.1844	0.509	0.1824	0.541
		der-1	0.1432	0.513	0.1571	0.545
		der-2	0.8969	0.229	0.8787	0.294
	1825-658	normal	0.1715	0.511	0.0509	0.543
		der-1	0.1384	0.513	0.2423	0.546
		der-2	0.1415	0.513	0.2338	0.546
	1524-658	normal	0.188	0.509	0.1693	0.54
		der-1	0.1427	0.513	0.146	0.545
		der-2	0.1456	0.513	0.1338	0.545
	3040-2784and 1825-658	normal	0.1698	0.511	0.1628	0.541
		der-1	0.1428	0.513	0.159	0.545
		der-2	0.1431	0.513	0.2064	0.545
	3040-1664and 1524-658	normal	0.1815	0.51	0.1696	0.541
		der-1	0.1431	0.513	0.1574	0.545
		der-2	0.962	0.141	0.8472	0.298
	3040-2784and 15244-658	normal	0.1782	0.51	0.3997	0.539
		der-1	0.8102	0.304	0.8652	0.354
		der-2	0.9209	0.202	0.8803	0.283
	3040-2784, 1825-1664and 1524-658	normal	0.1671	0.511	0.148	0.542
		der-1	0.1427	0.513	0.1592	0.545
		der-2	0.143	0.513	0.2073	0.545

PCR = principle component regression; PLSR = partial least square regression; R² = coefficient of determination; RMSEC = root mean square error of calibration; RMSEP = root mean square error of prediction. The yellow highlighted condition was selected for prediction of acid value.

Due to its capability to provide the highest of the coefficient of determination (R²) either in calibration and validation models and lowest values of root mean square error of calibration (RMSEC) and prediction (RMSEP), the first FTIR derivative spectra using PCR was selected for prediction of AV in frying oil. The wavenumbers used was 1524-658 cm^{-1} . The R² values obtained was 0.973 (in calibration) and 0.932 (in prediction or invalidation) with RMSEC

and RMSEP of 0.121 and 0.253. The high R² and low values of RMSEC and RMSEP indicated good accuracy and precision of models. Fig. 2 revealed the correlation between actual values of AV as determined using AOCS method and FTIR predicted values along with residual analysis (the difference between actual and predicted value). Residual values fall above and below zero (0) value, indicating that no systematic errors were observed during modeling.

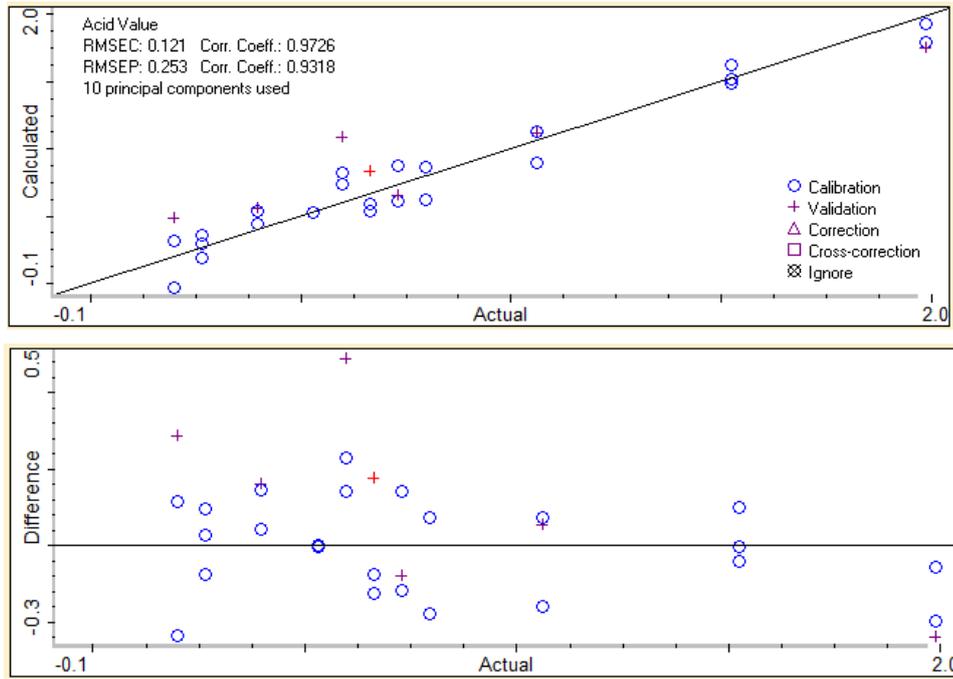


Fig. 2: The correlation between actual values of acid value and FTIR predicted values (above) along with residual analysis (below)

Table 3: The optimization of FTIR spectra in combination with multivariate calibration for prediction of iodine value

Multivariate Calibrations	Wavenumber (cm ⁻¹)	Spectra	Calibration		Validation	
			R ²	RMSEC	R ²	RMSEP
PCR	3059-659	normal	0.9608	3.09	0.9012	4.83
		der-1	0.7855	6.9	0.5293	9.14
		der-2	0.7814	6.96	0.4638	9.7
	1545-659	normal	0.9253	4.23	0.8378	6.95
		der-1	0.8744	5.41	0.6593	7.66
		der-2	0.9537	3.35	0.8213	5.93
	3059-2767and 1848-659	normal	0.9514	3.43	0.7914	6.92
		der-1	0.7838	6.92	0.5115	9.44
		der-2	0.7783	7	0.5657	8.74
	3059-1664and 1545-659	normal	0.9603	3.11	0.9002	4.85
		der-1	0.7864	6.89	0.5297	9.15
		der-2	0.78	6.98	0.4511	9.91
	3059-2767and 1545-659	normal	0.9456	3.65	0.8323	6
		der-1	0.8142	6.47	0.6858	7.38
		der-2	0.8181	6.41	0.6118	8.7
	3059-2767, 1848-1664and 1545-659	normal	0.9513	3.44	0.7862	7.09
		der-1	0.785	6.91	0.5104	9.47
		der-2	0.7775	7.01	0.5537	8.96
PLS	3059-659	normal	0.1362	11	0.045	10.1
		der-1	0.1452	11	0.1487	10.1
		der-2	0.1416	11	0.186	10.1
	1545-659	normal	0.1106	11.1	0.069	10.1
		der-1	0.1401	11	0.2899	10.1
		der-2	0.8357	6.12	0.7361	6.84
	3059-2767and 1848-659	normal	0.1329	11	0.0537	10.1
		der-1	0.1448	11	0.1518	10.1
		der-2	0.8661	5.57	0.6556	8.1
	3059-1664and 1545-659	normal	0.1358	11	0.0462	10.1
		der-1	0.1451	11	0.1486	10.1
		der-2	0.9005	4.85	0.6493	8.15
	3059-2767and 1545-659	normal	0.1373	11	0.0361	10.1
		der-1	0.1545	11	0.1291	10.1
		der-2	0.1471	11	0.2251	10.1
	3059-2767, 1848-1664and 1545-659	normal	0.1325	11.1	0.1548	10.1
		der-1	0.1448	11	0.1517	10.1
		der-2	0.8659	5.58	0.6252	8.48

PCR = principle component regression; PLSR = partial least square regression; R² = coefficient of determination; RMSEC = root mean square error of calibration; RMSEP = root mean square error of prediction. The yellow highlighted condition was selected for prediction of iodine value.

Similarly, table 3 and table 4 compiled the optimization results of FTIR spectroscopy in combination with multivariate calibration of PLSR and PCR for prediction of IV (table 3) and PV

(table 4). Again, the selection of FTIR spectra condition was based on the capability to provide the highest R² values and lowest RMSEC and RMSEP values.

Table 4: The optimization of FTIR spectra in combination with multivariate calibration for prediction of peroxide value

Multivariate calibrations	Wavenumber (cm ⁻¹)	Spectra	Calibration		Validation	
			R ²	RMSEC	R ²	RMSEP
PCR	3076-656	normal	0.9431	1.48	0.9508	2.07
		der-1	0.7208	3.09	0.7326	3.56
		der-2	0.734	3.03	0.7301	3.51
	1811-656	normal	0.9096	1.85	0.972	1.82
		der-1	0.7946	2.71	0.6914	3.94
		der-2	0.9347	1.59	0.7944	3.36
	1518-656	normal	0.905	1.9	0.9583	2.36
		der-1	0.9431	1.48	0.8578	2.64
		der-2	0.9312	1.63	0.8441	3.09
	3076-2783and 1811-656	normal	0.945	1.46	0.949	2.66
		der-1	0.7304	3.05	0.7469	3.48
		der-2	0.7381	3.01	0.7616	3.35
	3076-2783and 1518-656	normal	0.9301	1.64	0.9613	1.85
		der-1	0.7935	2.72	0.8596	2.57
		der-2	0.757	2.92	0.7703	3.32
3076-2783, 1811-1664and 1518-656	normal	0.9439	1.47	0.949	2.68	
	der-1	0.7303	3.05	0.7403	3.52	
	der-2	0.7163	3.12	0.7489	3.49	
PLS	3076-656	normal	0.1942	4.38	0.0389	5.4
		der-1	0.1829	4.39	0.1629	5.41
		der-2	0.1832	4.39	0.216	5.41
	1811-656	normal	0.1823	4.39	0.0205	5.42
		der-1	0.178	4.39	0.0919	5.42
		der-2	0.181	4.39	0.1302	5.41
	1518-656	normal	0.1875	4.39	0.0076	5.41
		der-1	0.1825	4.39	0.1024	5.41
		der-2	0.8456	2.38	0.7849	3.32
	3076-2783and 1811-656	normal	0.1854	4.39	0.0787	5.41
		der-1	0.1826	4.39	0.165	5.41
		der-2	0.929	1.65	0.8422	3.01
	3076-2783and 1518-656	normal	0.1885	4.38	0.1431	5.41
		der-1	0.1865	4.39	0.1741	5.41
		der-2	0.7342	3.03	0.6517	3.92
3076-2783, 1811-1664and 1518-656	normal	0.1838	4.39	0.1004	5.42	
	der-1	0.1826	4.39	0.1652	5.41	
	der-2	0.869	2.21	0.8153	3.21	

PCR = principle component regression; PLSR = partial least square regression; R² = coefficient of determination; RMSEC = root mean square error of calibration; RMSEP = root mean square error of prediction. The yellow highlighted condition was selected for prediction of peroxide value.

Finally, IV was best predicted using PCR with normal FTIR spectra at the combined wavenumbers region of 3076-2783and 1811-656 cm⁻¹. PCR using normal spectra at combined wavenumbers region of 3076-2783and 1811-656 cm⁻¹ was also selected for prediction of PV. Fig. 3 and fig. 4 showed a correlation between actual values of IV and

PV as determined using AOCS method and FTIR predicted values. The high R² values and low values of RMSEC and RMSEP indicated that FTIR spectroscopy is accurate and precise model for prediction of IV and PV, and could be used as an alternative method toward standard titrimetric method.

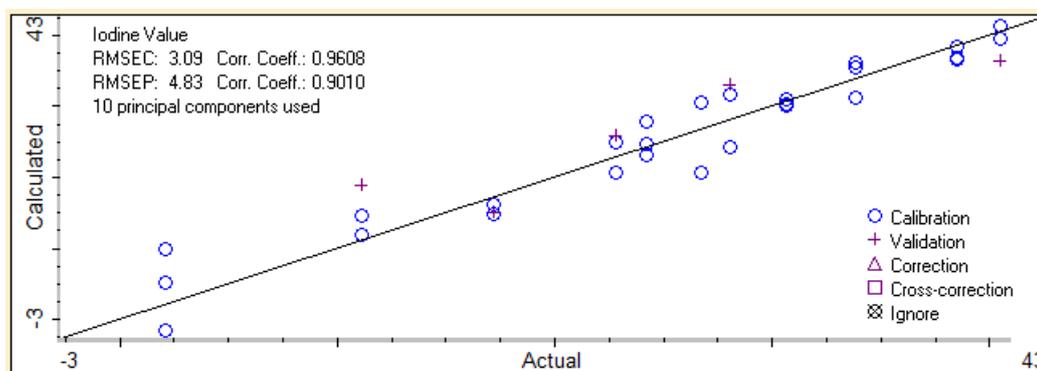


Fig. 3: The correlation between actual values of iodine value and FTIR predicted values

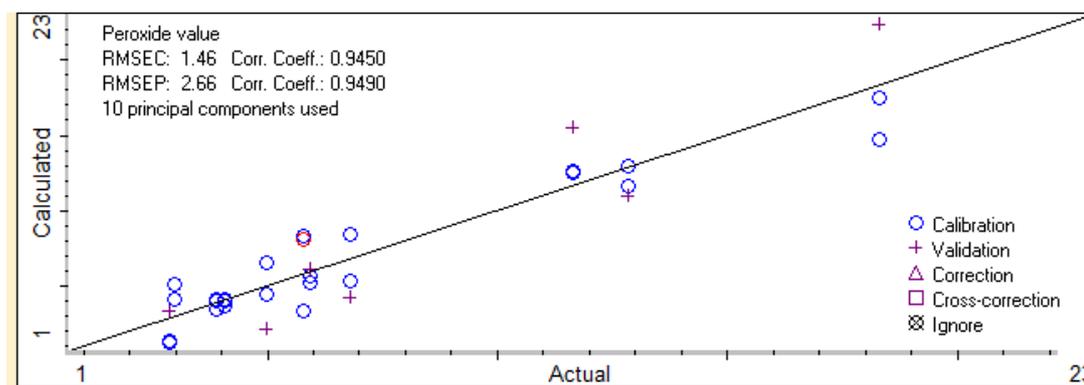


Fig. 4: The correlation between actual values of peroxide value and FTIR predicted values

CONCLUSION

FTIR spectroscopy in combination with principle component regression (PCR) offered a reliable and fast method for prediction of AV, IV, and PV in frying oils. Using optimized condition based on high values of R^2 and low value of calibration and validation errors, FTIR spectroscopy could be used successfully for prediction of AV, IV, and PV. The high R^2 values and low values of RMSEC and RMSEP indicated that FTIR spectroscopy in combination with PCR is an accurate and precise model for prediction of AV, IV and PV, and could be used as an alternative method toward standard titrimetric method.

GRANT INFORMATION

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AUTHORS CONTRIBUTION

SP, M, and AR designed research, performed research activities, analysed data, prepared manuscript and made critical thinking on the manuscript.

CONFLICTS OF INTERESTS

All authors have none to declare

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