

APPLICATION OF FOURIER TRANSFORM INFRARED SPECTROSCOPY FOR DETERMINING SOME PARAMETERS OF PALM OIL

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Introduction

Malaysia is the largest producer and exporter in palm oil industry. Quality control system of palm oil and its fractions turns out to be more and more important. However, many analytical methods based on AOCS and IUPAC to measure some parameters of quality of palm oil are not very practical (AOCS, 1995). Fourier transform infrared spectroscopy has become widely used for the determination of some parameters of edible oils and fats (van de Voort, 1992; van de Voort, 1994). It has largely replaced manual analysis by analytical methods, improving efficiency, and reducing the requirement for skilled labour and the use of hazardous chemicals without sacrificing accuracy (Stuart, 1996). Therefore the objectives of this study were to determine the iodine value (IV) of palm oil and its products, the free fatty acid (FFA) in palm olein, the peroxide value (PV) of oxidised palm olein and the anisidine value (AnV) of thermally oxidised palm olein.

Materials and Methods

Materials: RBD palm olein, superolein, palm oil, palm stearin, oleic acid. **Methods:** a few drops of each sample were placed on the demountable cells. The cells were mounted in a cell holder in the FTIR spectroscopy and the scanning of each sample was carried out. These spectra were ratioed against background air spectrum. All standards were scanned in duplicate in region of 4000 to 400 cm^{-1} . A partial-least-squares (PLS) analysis was chosen to develop a calibration model. Correlation spectra, which relate spectral changes to the value of the variable of interest, were generated and examined to identify spectral features that correlate with the chemical data for samples. Calibration was derived and optimised to generate a predictive model for determination some parameters. The calibration routine includes a validation procedure, which provides statistical parameters indicative of the predictive capability of the calibration model. The accuracy of the validation step was assessed according to the standard error of prediction (SEP) and the coefficient of determination (R^2).

Results and Discussion

The chemical results of some parameters obtained from the AOCS method and the spectral data obtained from scanning the samples by FTIR spectroscopy were used together to predict the FTIR results. In IV determination, the spectral region of a calibration set that covering a range of 27.9 to 65.3 IV units between 3050 and 2984 cm^{-1} , corresponding to the absorption band of =C-H cis stretching vibration was used to build the PLS calibration model for the prediction of IV. A validation approach of this model yielded a good R^2 of 0.9995 and a SEP of 0.151. A set of palm olein samples that covers a wide range of FFA (0.08-1.04%) was used as the calibration standard. A PLS calibration model for the prediction of FFA was developed based on the spectral range of C=O stretching of FFA of 1728-1662 cm^{-1} . The R^2 and SEP yielded were 0.997 and 0.017% FFA units. For accuracy, the mean difference gave a value of 0.00016, with FTIR method giving the higher prediction of FFA of palm olein than chemical method. In determining PV of palm olein, the samples, the samples having PV range of 3.52 to 9.86 was used to construct the calibration model. For this calibration set, the spectral region used in the calibration was set to include all the data from 3082 to 3470 cm^{-1} . The SEP obtained was 0.172 PV. The SEP obtained can be considered a measure of the accuracy of the FTIR PV method because it relates predicted PV to chemical PV. In terms of reproducibility, the duplicate FTIR analysis had a standard deviation of the difference (SDD) of 0.02 PV, compared to an SDD of 0.05 PV for duplicate chemical analyses. The SDD of the chemical method was higher, indicating that the FTIR method is superior in producing consistent results for anyone sample. In the AnV determination of palm olein, a FTIR calibration model was obtained, using the two wavelength regions (2747 to 2619 cm^{-1} and 1715 to 1673 cm^{-1}). When the validation set predicted with the calibration model, the SEP was 0.51, the R^2 was 0.990 and the mean difference and standard deviation of difference for accuracy were 0.0864 and -0.0997, respectively. In terms of reproducibility, both the chemical and FTIR results have comparable mean differences and standard deviations.

Conclusions

In this study, the determination of IV, FFA, PV, AnV of palm oil and its products by using a transmission cell approach/FTIR spectroscopy and PLS analysis gave satisfactory results comparing to the chemical method with good accuracy.

References

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