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In situ Real-Time Multivariate Analysis of Methanolysis Monitoring of Sunflower Oil Using FTIR

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Abstract : The combination of world population and the third industrial revolution led to high demand for fuels. On the other hand, the decrease of global fossil 8fuels deposits and the environmental air pollution caused by these fuels has compounded the challenges the world faces due to its need for energy. Therefore, new forms of environmentally friendly and renewable fuels such as biodiesel are needed. The primary analytical techniques for methanolysis yield monitoring have been chromatography and spectroscopy, these methods have been proven reliable but are more demanding, costly and do not provide real-time monitoring. In this work, the in situ monitoring of biodiesel from sunflower oil using FTIR (Fourier Transform Infrared) has been studied; the study was performed using EasyMax Mettler Toledo reactor equipped with a DiComp (Diamond) probe. The quantitative monitoring of methanolysis was performed by building a quantitative model with multivariate calibration using iC Quant module from iC IR 7.0 software. 15 samples of known concentrations were used for the modelling which were taken in duplicate for model calibration and cross-validation, data were pre-processed using mean centering and variance scale, spectrum math square root and solvent subtraction. These pre-processing methods improved the performance indexes from 7.98 to 0.0096, 11.2 to 3.41, 6.32 to 2.72, 0.9416 to 0.9999, RMSEC, RMSECV, RMSEP and R2Cum, respectively. The R² value of 1 (training), 0.9918 (test), 0.9946 (cross-validation) indicated the fitness of the model built. The model was tested against univariate model; small discrepancies were observed at low concentration due to unmodelled intermediates but were quite close at concentrations above 18%. The software eliminated the complexity of the Partial Least Square (PLS) chemometrics. It was concluded that the model obtained could be used to monitor methanol of sunflower oil at industrial and lab scale.

Keywords : biodiesel, calibration, chemometrics, methanolysis, multivariate analysis, transesterification, FTIR
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