Multivariate Calibration and Near Infrared Spectroscopic Models for Predicting Biodiesel Quality

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Biodiesel is gaining more importance as an attractive fuel due to the enormous consumption of energy in the world. It can easily be isolated from transesterification reactions of vegetable oils or fats with alcohols in the presence of catalyst [1]. The quality of final product is an important issue and therefore a lot of techniques have been developed. Near infrared (NIR) spectroscopy has recently become an alternative method to the conventional analytical methods such as chromatography.

In this study, laboratory scaled biodiesel was produced from two different vegetable oils (sunflower and corn oil). In addition, the mixture of vegetable oils and a mono alcohol with their corresponding biodiesel were prepared to represent the reaction media for sunflower and corn oil respectively. Development of multivariate calibration methods are carried following the near infrared spectroscopic measurements. Since NIR measurements include several spectral overlaps due to the multicomponent media (Figure 1) the data should be handled using multivariate calibration techniques rather than univariate approaches. Multivariate analysis offers the advantage of using several wavelengths in order to build linear calibration models but some of the wavelengths in the whole spectrum may sometimes contain nonlinear responses and even noise which distorts the success of models. Cases like this may be improved by a wavelength selection step prior to model building. Consequently, in this study, calibration models of each component were built by a genetic algorithm based inverse least squares method (GILS) [2]. The results demonstrated that, NIR spectroscopy can be used as a quantitative method without any pretreatment in the determination of the quality of biodiesel in conjunction with multivariate calibration methods.

**Figure 1.** NIR spectra of biodiesel, reactants and their mixtures.

References