Calibration method for the determination of the FAME and HVO contents in fossil diesel blends using NIR spectroscopy

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Abstract

According to the European standard EN590 for automotive diesel fuel, no additional labeling is required for the diesel fuel additives, such as bio fuels, including the biodiesel (FAME) blended up to 7 % (V/V) and renewable diesel (HVO) with undefined blending ratio. However, the information about the bio fuels' content in diesel fuel blends is an important aspect of the fuels analysis. This work presents a calibration method development for quantification of FAME and HVO contents in diesel fuel blends within the analytical range of 0 – 10 % (V/V) and 0 – 20 % (V/V) respectively using near-infrared spectroscopy. The development of the calibration method is based on partial least squares (PLS) regression method for multivariable data analysis and construction of the calibration models. The constructed PLS models obtained prediction results for all diesel fuel blends with root mean square error of prediction (RMSEP) values of 2.66 % (V/V) for the renewable diesel content quantification and 0.18 % (V/V) for quantification of the biodiesel content, concluding that the calibration method is suitable for practical laboratory applications.

Keywords: Diesel fuel blends, Biodiesel, Renewable diesel, Near-infrared spectroscopy, Partial least squares regression

1. Introduction

The European standard EN 590 for automotive fuels, concerning diesels, states that the use of the diesel fuel additives is allowed for automotive diesel fuel. [1] Such additives may include the fuels developed from alternative to fossil feedstock, renewable feedstock, such as fats and oils. Nowadays, the major diesel fuel additives derived from renewable biological sources are biodiesels and renewable diesels. These fuels have different compositions and properties, due to the different processes of fuels' production, even if the used feedstock is the same. [2]

Biodiesels are defined as fatty acid methyl ester (FAME) fuels. Biodiesels production process is based on the transesterification reaction, where organic feedstock, such as animal fat or vegetable oils, reacts with alcohols in the presence of a catalyst to produce fatty acid alkyl esters. Today, the dominant renewable feedstock for biodiesel production in Europe is rapeseed oil, from which rapeseed methyl ester (RME) fuel is derived. The other sources used for biodiesel production include, e.g., soybean, sunflower and palm oils, as well as animal fat, algae and others. [3] According to the EN 590 standard, current automotive fuel diesel "may contain up to 7 % (V/V) of FAME complying

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Abbreviations used in this article: AFME – Animal fat methyl ester; CNUM – Number of PLS components; DFO – Diesel fuel oil; FAME – Fatty acid methyl ester; HVO – Hydrotreated vegetable oil; NIR – Near-infrared; PLS – Partial least squares; PRESS – Prediction residual sum of squares; R^2 – Coefficient of determination; RME – Rapeseed methyl ester; RMSECV – Root mean squared error of cross validation; RMSEP – Root mean square error of prediction; SNV – Standard normal variate