World Academy of Science, Engineering and Technology
International Journal of Energy and Environmental Engineering
Vol:9, No:12, 2015

Simultaneous Determination of Six Characterizing/Quality Parameters of Biodiesels via 1H NMR and Multivariate Calibration

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Abstract : The characterization and the quality of biodiesel samples are checked by determining several parameters. Considering a large number of analysis to be performed, as well as the disadvantages of the use of toxic solvents and waste generation, multivariate calibration is suggested to reduce the number of tests. In this work, hydrogen nuclear magnetic resonance (1H NMR) spectra were used to build multivariate models, from partial least squares (PLS) regression, in order to determine simultaneously six important characterizing and/or quality parameters of biodiesels: density at 20 ºC, kinematic viscosity at 40 ºC, iodine value, acid number, oxidative stability, and water content. Biodiesels from twelve different oils sources were used in this study: babassu, brown flaxseed, canola, corn, cottonseed, macauba almond, microalgae, palm kernel, residual frying, sesame, soybean, and sunflower. 1H NMR reflects the structures of the compounds present in biodiesel samples and showed suitable correlations with the six parameters. The PLS models were constructed with latent variables between 5 and 7, the obtained values of r(cal) and r(val) were greater than 0.994 and 0.989, respectively. In addition, the models were considered suitable to predict all the six parameters for external samples, taking into account the analytical speed to perform it. Thus, the alliance between 1H NMR and PLS showed to be appropriate to characterize and evaluate the quality of biodiesels, reducing significantly analysis time, the consumption of reagents/solvents, and waste generation. Therefore, the proposed methods can be considered to adhere to the principles of green chemistry.

Keywords : biodiesel, multivariate calibration, nuclear magnetic resonance, quality parameters
Conference Title : ICBB 2015 : International Conference on Biofuels and Bioenergy
Conference Location : Paris, France
Conference Dates : December 30-31, 2015