Abstract

Using overtone regions to determine biodiesel content in diesel/biodiesel blends adulterated with vegetable oils

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Introduction

In Brazil, the commercial use of blended biodiesels has been obligatory by law since 2008. There is now a need to develop low cost instrumentation to determine the biodiesel content of these blends accurately. Overtone regions could be useful for this purpose.

Materials and Methods

Blends were prepared using different samples of diesel fuel and different oilseeds, animal fats and their respective esters. A mixture design with central point for each biodiesel type, including internal points, was used to prepare these blends. A data set of 124 samples, with ester and vegetable oil content ranging from 0.0 to 10.0% v/v, was obtained. Spectra were obtained using three different optical paths: 10 mm (9000–6300 cm^{-1}), 20 mm (11600–6300 cm^{-1}) and 50 mm (7500–6300 cm^{-1}). Computations were performed using both The Unscrambler (v. 9.5) and Matlab (v. 6.5) software. Models were obtained using Partial Least Squares Regression (PLS) and Multiple Linear Regression (MLR) techniques and two methods of variable selection: (1) Successive Projections Algorithm (SPA/MLR), and (2) significant regression coefficients using the jack-knife algorithm (PLS/JK).

Results and Discussion

For the 10, 20 and 50 mm optical paths and using overtone bands, the RMSEP values obtained with the PLS-JK models were 0.38% v/v, 0.45% v/v and 0.20% v/v respectively. SPA/MLR models for the same optical paths were 0.07% v/v, 0.12% v/v and 0.12% v/v respectively. In general, the results point to SPA/MLR as the better modeling strategy. It is worth noting that this strategy is simpler and uses a smaller number of spectral variables (e.g. twelve spectral variables).

Conclusion

The potential of overtone regions to predict biodiesel content in diesel/biodiesel blends, in the range from 0.0% to 10.0% v/v, considering the possible presence of raw oil as a contaminant was confirmed by the systematic study performed varying the optical paths.

Reference paper as:
F. Vasconcelos, P.S. Júnior, M. F. Pimentel, M. Pontes and C. Pereira (2012).Using overtone regions to determine biodiesel content in diesel/biodiesel blends adulterated with vegetable oils (abstract), in: Proceedings of the 15th International Conference on Near Infrared Spectroscopy, Edited by M. Manley,C.M. McGoverin, D.B. Thomas and G. Downey, Cape Town, South Africa, p. 206.