

Predicting percent composition of blends of biodiesel and conventional diesel using gas chromatography-mass spectrometry, comprehensive two-dimensional gas chromatography-mass spectrometry, and partial least squares analysis.

Karisa M. Pierce* and Stephen P. Schale

Abstract

The percent composition of blends of biodiesel and conventional diesel from a variety of retail sources were modeled and predicted using partial least squares analysis (PLS) applied to gas chromatography-total-ion-current mass spectrometry (GC-TIC), gas chromatography-mass spectrometry (GC-MS), comprehensive two-dimensional gas chromatography-total-ion-current-mass spectrometry (GCxGC-TIC) and comprehensive two-dimensional gas chromatography-mass spectrometry (GCxGC-MS) separations of the blends. In all four cases, the PLS predictions for a test set of chromatograms were plotted versus the actual blend percent composition. The GC-TIC plot produced a best-fit line with slope = 0.773 and y-intercept = 2.89, and the average percent error of prediction was 12.0%. The GC-MS plot produced a best-fit line with slope = 0.864 and y-intercept = 1.72, and the average percent error of prediction was improved to 6.89%. The GCxGC-TIC plot produced a best-fit line with slope = 0.983 and y-intercept = 0.680, and the average percent error was slightly improved to 6.16%. The GCxGC-MS plot produced a best-fit line with slope = 0.980 and y-intercept = 0.620, and the average percent error was 6.12%. The GCxGC models performed best presumably due to the multidimensional advantage of higher dimensional instrumentation providing more chemical selectivity. All the PLS models used 3 latent variables. The chemical components that differentiate the blend percent compositions are reported.

*Corresponding Author:

Karisa M. Pierce, Ph.D.

Assistant Professor

Department of Chemistry

Seattle Pacific University

206-281-2102 office

206-281-2882 fax

pierck1@spu.edu

3307 Third Avenue West, Suite 205

Seattle, WA 98119-1950

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