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A comparison of different strategies in multivariate regression models for the direct determination of Mn, Cr, and Ni in steel samples using laser-induced breakdown spectroscopy

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Abstract

Laser-induced breakdown spectroscopy (LIBS) analysis was carried out on eleven steel samples to quantify the concentrations of chromium, nickel, and manganese. LIBS spectral data were correlated to known concentrations of the samples using different strategies in partial least squares (PLS) regression models. For the PLS analysis, one predictive model was separately generated for each element, while different approaches were used for the selection of variables (VIP: variable importance in projection and iPLS: interval partial least squares) in the PLS model to quantify the contents of the elements. The comparison of the performance of the models showed that there was no significant statistical difference using the Wilcoxon signed rank test. The elliptical joint confidence region (EJCR) did not detect systematic errors in these proposed methodologies for each metal.

Keywords: partial least squares regression (PLS); selection of variables; laser-induced breakdown spectroscopy (LIBS); steel samples; figures of merit.

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