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Quantitative Analysis of Steel using Laser-Induced Breakdown Spectroscopy and Chemometrics

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Laser-Induced Breakdown Spectroscopy (LIBS) has been applied for multielemental analysis of solid steel samples containing several major elements (Fe, Mn, Si, Cu, Ni, Cr, Mo, W, V and Co) using a multivariate model. A review of the literature reveals that improving the accuracy and the robustness of the quantitative analysis of these elements presents a great interest, in particular, for industrial on-line analysis. Indeed, composition changes of the major elements (e.g. from 0.1 up to $20\% \binom{m}{m}$) will induce significant changes in the observed signal in LIBS. Therefore, the observed relationship between signal and concentration might become scattered deteriorating the quality of the regression line. These "indiscriminate" behaviors of the analytical signals, in traditional univariate calibration, are called matrix effects. It is well known in the scientific community that a matrix-matched calibration standard can be used to overcome these problems. The use of a matrix-matched calibration requires additional experimental data and treatment to achieve reliable quantitative analysis. This indicates that traditional univariate calibration, which is generally used in LIBS, may not be an appropriate choice for this application where large composition changes in the matrix are present. In the present work, we show that the post-processing chemometrics applied to LIBS signals presents a great potential. The results obtained by using a multivariate model showed that it allowed correcting the matrix effects and consequently significantly improving the quality of the quantitative analysis.