LIBS, from research to Industry
P077. LIBS strategy calibration by using Artificial Neural Network
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A relevant feature of LIBS is its versatility, which permits to perform analysis in situ, by use of a compact instrumentation. Especially for soil analysis, the elemental determination in situ can represent a great saving of time, besides reducing the costs associated to transport and preservation of samples, conventional laboratorial analysis and residues generation. A quantitative methodology to perform elemental analysis in situ of soil samples can represent a great contribution for precision agriculture development.

LIBS technique have been easily employed for qualitative analysis, nevertheless it still requires certain effort to perform quantitative analysis, since calibration represents a difficult issue in the development of LIBS methods. It occurs because LIBS signals for the same element often depends on the matrix in which it is embedded. The sensibility to the matrix effects and their influence on the results is an unsolved problem related to LIBS [1]. Thus, an alternative for LIBS calibration methods would be the use of certificate reference materials. However, for LIBS measurements the sampling mass are of micrograms order (< 20 µg), and there is no reference materials with certificated properties for inferior masses of 0.1 mg [2]. In this work calibration strategies based on artificial neural networks (ANN) were considered. Sixty samples of Brazilian soils with elemental composition pre-determined by 90 laboratories were averaged and used for the calibration set. The same samples were submitted to analyses in a commercial portable LIBS system operating with a single pulse of laser and four CCD detectors for date aquisition from 190 nm to 1000 nm. The initial experiments were conducted for copper and the spectra acquired from 190 nm to 400 nm were used. The data were normalized to improve the ANN accuracy. The ANN type MultiLayer Perceptron (MLP) [3] was trained and a 10-fold cross-validation methodology was applied to evaluate its prediction performance. The results show that ANN is a promising chemometric technique for LIBS methods.