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Challenges in the quantification of nutrients in soils using laser-induced breakdown spectroscopy – a case study with calcium

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Abstract

The quantification of the elemental content in soils with laser-induced breakdown spectroscopy (LIBS) is challenging because of matrix effects strongly influencing the plasma formation and LIBS signal. Furthermore, soil heterogeneity at the micrometre scale can affect the accuracy of analytical results. In this paper, the impact of univariate and multivariate data evaluation approaches on the quantification of nutrients in soil is discussed. Exemplarily, results for calcium are shown, which reflect trends also observed for other elements like magnesium, silicon and iron. For the calibration models, 16 certified reference soils were used. With univariate and multivariate approaches, the calcium mass fraction in 60 soils from different testing grounds in Germany were calculated. The latter approach consisted of a principal component analysis (PCA) of adequately pre-treated data for classification and identification of outliers, followed by partial least-squares regression (PLSR) for quantification. For validation, the soils were also characterised with inductively coupled plasma optical emission spectroscopy (ICP OES) and X-ray fluorescence (XRF) analysis. Deviations between the LIBS quantification results and the reference analytical results are discussed.

Keywords: laser-induced breakdown spectroscopy (LIBS); soil; multivariate data analysis; principal component analysis (PCA); partial least squares regression (PLSR)

1 Introduction

Site-specific fertility management represents a significant improvement of efficient cultivation of agricultural cropland. Therefore, affordable and extensive mapping methods are needed. A conventional and reliable method for the determination of element concentrations in soils is inductively coupled plasma optical emission spectroscopy (ICP OES). However, for the measurement with ICP OES time-consuming soil digestion is necessary [1]. Digestion

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