Feasibility for chemometric energy dispersive X-ray fluorescence and scattering (EDXRFS) spectroscopy method for rapid soil quality assessment

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Date: 2011

Abstract

Soil quality assessment (SQA) is important for modulating agricultural productivity and thus requires simple and rapid analysis of soil (macro & micro) nutrients (here called soil quality indicators – SQIs). We report proof of concept of a chemometricsassisted energy dispersive X-ray fluorescence and scattering (EDXRFS) spectroscopy technique for direct rapid analysis of SQIs. The EDXRFS method exploits, in addition to fluorescence, the X-ray scatter peaks obtained non-invasively from soils to develop a calibration strategy for quantitative analysis of SQIs in model clay soils doped with micronutrients (Fe, Cu, and Zn) and macronutrients (NO3 , SO4 2 , and H2PO4). The soil samples and certified reference materials IAEA Soil-7 and IAEA Soil-1 (used to build spectral library for soil classification) were irradiated at various live times (to simulate different signal-to-noise ratios of analyze signals and analysis speed) in a teflon holder and were analyzed using a 109Cd-excited XRF spectrometer. Principal components analysis was used for spectral data compression and pattern recognition (including for those SQI spectral signatures without any visibly discernible characteristic X-ray lines), whereas partial least squares regression and artificial neural networks were used to build a calibration and quantitative analysis strategy. The method furnishes soil micronutrient and macronutrient information simultaneously and rapidly (t = 200 s). To the best of the authors' knowledge, this is the first time that an XRF method has demonstrated spectroanalytical potential for quantitative macronutrients analysis in soils applicable to routine SQA. Coupling EDXRFS with multivariate chemometrics enables rapid and reliable assessment of chemical SQIs.