Global soil characterization with VNIR diffuse reflectance spectroscopy

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Abstract

There has been growing interest in the use of diffuse infrared reflectance as a quick, inexpensive tool for soil characterization. In studies reported to date, calibration and validation samples have been collected at either a local or regional scale. For this study, we selected 3768 samples from all 50 U.S. states and two tropical territories and an additional 416 samples from 36 different countries in Africa (125), Asia (104), the Americas (75) and Europe (112). The samples were selected from the National Soil Survey Center archives in Lincoln, NE, USA, with only one sample per pedon and a weighted random sampling to maximize compositional diversity. Applying visible and near-infrared (VNIR) diffuse reflectance spectroscopy (DRS) to airdry soil (<2 mm) with auxiliary predictors including sand content or pH, we obtained validation root mean squared deviation (RMSD) estimates of 54 g kg^{-1} for clay, 7.9 g kg^{-1} for soil organic C (SOC), 5.6 g kg_1 for inorganic C (IC), 8.9 g kg^{-1} for dithionate–citrate extractable Fe (FEd), and 5.5 cmolc kg^{-1} for cation exchange capacity (CEC) with NH4 at pH=7. For all of these properties, boosted regression trees (BRT) outperformed PLS regression, suggesting that this might be a preferred method for VNIR-DRS soil characterization. Using BRT, we were also able to predict ordinal clay mineralogy levels for montmorillonite and kaolinite, with 88% and 96%, respectively, falling within one ordinal unit of reference X-ray diffraction (XRD) values (0–5 on ordinal scale). Given the amount of information obtained in this study with ~4 $x10^3$ samples, we anticipate that calibrations sufficient for many applications might be obtained with large but obtainable soil-spectral libraries (perhaps 104–105 samples). The use of auxiliary predictors (potentially from complementary sensors), supplemental local calibration samples and theoretical spectroscopy all have the potential to improve predictions. Our findings suggest that VNIR soil characterization has the potential to replace or augment standard soil characterization techniques where rapid and inexpensive analysis is required.

Keywords: Diffuse reflectance spectroscopy; VNIR; PLS regression; Clay mineralogy; Boosted regression trees; Soil characterization

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