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Characterizing soils using a portable X-ray fluorescence spectrometer: 1. Soil texture

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ABSTRACT

The development of new technologies for use in field soil survey has produced powerful new quantitative tools for assessing soil physicochemical properties *in-situ*. One such technology, portable X-ray fluorescence (PXRF) spectrometry, has shown considerable promise in evaluating elemental concentrations in soils for a wide variety of applications. Less research is available on how PXRF can be applied to quantify soil physical properties (e.g. soil texture). This study evaluated the feasibility of predicting soil clay and sand contents from PXRF data on 584 soil samples collected from highly diverse regions of Louisiana and northeastern New Mexico (Capulin Volcano National Monument), USA. An Innov-X Delta Premium PXRF was used to sequentially scan soil samples under both field and laboratory conditions and assess 15 elements (K, Ca, Ti, Cr, Mn, Fe, Co, Cu, Zn, As, Rb, Sr, Zr, Ba, and Pb). Elemental concentrations were then related to soil textural data processed through traditional laboratory methods with multiple linear regression. Among all elements evaluated, Fe and Rb showed particular significance for soil textural prediction. The regression models for sand and clay contents of both study sites were strongly correlated to soil textural separates with PXRF-soil texture R^2 of 0.862, 0.959, 0.892, and 0.780 for Louisiana sand and clay, and Capulin sand and clay, respectively. Independent validation sub-datasets confirmed that PXRF readings can be used to estimate soil textural parameters with high R^2 values of 0.854, 0.682, 0.975, 0.891, 0.875, and 0.876, and low RMSE values of 5.53%, 5.92%, 2.68%, 6.26%, 5.43%, and 2.66%, for Louisiana sand, silt, and clay and Capulin sand, silt, and clay, respectively. The RMSE values of clay are substantially lower than those reported in previous studies using other proximal sensing techniques. While regional differences may require localized standardization of the PXRF with a unique combination of elements germane to the study area, PXRF shows considerable promise as a technique for rapidly assessing soil textural separates *in-situ*.

1. Introduction

Traditional soil survey and physiochemical laboratory analysis of soil samples has been the standard method of expanding our understanding of soils. However, these techniques are generally time consuming and cost prohibitive (Viscarra Rossel et al., 2010; Waiser et al., 2007). The demand for good quality, inexpensive and high-resolution soil information has been growing recently in areas such as precision agriculture and land planning. Thus, the development of more time- and cost-efficient quantitative methods of soil analysis and information gathering has become a priority (Viscarra Rossel et al., 2010).

Many new techniques and concepts have been promising and successful in predicting soil properties in unvisited areas based on existing documented information. For example, with advances of computer science, remote and proximal sensing, digital soil mapping has been extensively reported as an efficient tool to infer patterns of soil across various spatial and temporal scales (Boettinger et al., 2010; Carré et al., 2007; Grunwald, 2009; Hartemink et al., 2008; Lagacherie et al., 2006). New instruments incorporate sensors that are smaller, faster, more accurate and more intelligent for obtaining soil information. For instance, visible near-infrared diffuse reflectance spectroscopy (VNIR-DRS) has been reported as an effective tool to measure a variety of soil properties including clay (Bricklemyer and Brown, 2010; Brown, 2007; Waiser et al., 2007), soil organic carbon (Ge et al., 2011; Morgan et al., 2009; Sankey et al., 2008), color (Viscarra Rossel et al., 2009; Viscarra Rossel and Chen, 2011), soil water (Zhu et al., 2010), and soil composition and mineralogy (Serbin et al., 2009). Over the last fifty years, x-ray fluorescence (XRF) spectrometry has evolved from a manual technique to an automated tool to provide comprehensive, quantitative analytical data for scientists and industrialists (Potts and West, 2008). In the last 20 years, portable x-ray fluorescence (PXRF) spectrometry has been developed and improved greatly and is recently commercially available by several manufacturers (Potts and West, 2008). However, as one of the newly emerged techniques, PXRF has yet to be utilized by most soil scientists.

Both XRF and PXRF provide a multi-element analytical approach to routine non-destructive and non-invasive analysis of many materials including soil and sediments with minimal sample preparation (Herpin et al., 2002; Potts et al., 2002; Stephens and Calder, 2004). The most attractive feature of XRF is its wide dynamic range, from

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parts-per-million (ppm or mg kg^{-1}) to 100%, for many elements present in a given sample (Hettipathirana, 2004). Portable x-ray fluorescence inherited the advantages of XRF, and is one of a few analytical techniques that are capable of *in-situ* analysis, providing chemical composition of a sample in a short period of time (30–120 s) to the operator in the field (Potts, 2008). The major concern of PXRF performance is the non-homogeneity of efficiency for different elements (Kalnicky and Singhvi, 2001; Migliori et al., 2011; Weindorf et al., 2011), which is still being improved upon by users and manufacturers. Nevertheless, PXRF is able to offer acceptable quantitative results regarding chemical composition of the studied materials, as reported by VanCott et al. (1999) and Weindorf et al. (2008).

The variations of chemical composition of the soil reflect both the parent materials and the weathering status and intensity of pedogenesis, which then produces a variety of soil properties including soil texture, color, and mineralogical composition (Sparks, 2003; van Breemen and Buurman, 2002). Most previous applications of PXRF in soil science were focused on the determination of heavy metal concentrations for environmental assessment, screening, monitoring, and mitigation (Lawryk et al., 2009; Palmer et al., 2009; Radu and Diamond, 2009; Stallard et al., 1995; Weindorf et al., 2011). Few, if any, studies have attempted to infer soil properties other than trace element concentrations by using PXRF.

In this study, we hypothesize that soil textures in a relatively homogeneous environmental setting (e.g., regional scale) correlate strongly with soil chemical composition and therefore can be predicted from the direct elemental readings of PXRF. This study examines the relationship between soil texture and chemical composition in both a large area (the State of Louisiana) and a small area (Capulin Volcano National Monument, New Mexico). The major objective of this study is to build a simple regression model which can predict the percentages of sand, silt, and clay based on PXRF readings of the soil and can therefore be used to provide soil textural information for fieldwork.

2. Materials and methods

2.1. Description of the study sites

Louisiana consists of 112,825 km^2, extending from the Gulf Coast inland about 610 km. Elevation of the state ranges from 163 m to −2 m (USGS, 2010). The state is dissected by numerous river systems, most notably by the Mississippi River, Red River, and Ouachita River. About 55% of the surface of Louisiana is underlain largely by geologically young sediment; Holocene deposits associated with alluvium of the major rivers and coastal marsh deposits. Most of the rest of the state's surface (25%) consists of strata of Tertiary materials in northwestern and north Louisiana, ranging in age from Paleocene to Pliocene (Louisiana Geological Survey Staff, 2008). The climate of Louisiana is moist and subtropical. Average annual temperatures range from 17 °C in the northern part of the state to 22 °C along parts of the coast. Average annual rainfall ranges from 119 cm in the northwestern part of the state to 180 cm in isolated areas north of Lake Ponchartrain. The soils of Louisiana are grouped into six major soil areas based on landscape setting and parent material, i.e., coastal plain, flatwoods, coastal prairie, loess hills, recent alluvium, and coastal marsh (Amacher et al., 1989). Soil temperature regimes in Louisiana are thermic and hyperthermic, and soil moisture regimes are udic or aquic (Weindorf, 2008). Smectite, illite, and kaolinite are the three dominant clay minerals in the state, varying considerably in their relative abundances (Roberts, 1985).

Capulin Volcano National Monument is located in Union County, northeastern New Mexico, covering an area of ~324 ha. The volcano formed approximately 62,000 years ago and represents the youngest volcano in the Raton Clayton Volcanic Field (USDI-NPS, 2008). The cone of the volcano rises 396 m from the plain, with a base of 6.4 km in circumference and a crater of 126 m deep and 442 m in diameter (USDI-NPS, 2008). The top of the cone reaches an altitude of 2495 m above sea level (USDI-NPS, 2008). The Monument has a mild, arid or semiarid, continental climate characterized by light precipitation totals (~38.4 cm annually), low relative humidity (~65% on average), and a relatively large temperature range with average annual highs and lows of 19.4 °C and 4.2 °C, respectively (NOAA-NWS, 2008). The Monument is naturally vegetated with woody species, prairie grass species, and various cacti, yucca, and wildflower species. The National Cooperative Soil Survey and USDA-NRCS provide only limited soil data for the Monument. Specifically, three mapping units are noted within the soil survey geographic (SSURGO) data in the sampling area: the Bandera Association 'Bd', the Fallsam Rock Outcrop Complex 'Fr', and Brier-Rock outcrop complex 'Lr' (Table 1), which account for ~60%, 35%, and 5% of the soils mapped on the Monument, respectively (Soil Survey Staff, 2008). The information also includes substantial uncertainty (Weindorf and Zhu, 2010). The 'Bd' mapping unit contains ~65% Bandera soil, ~20% cinder land and ~15% other soils, while the 'Fr' mapping unit consists of ~50% Fallsam soil, ~20% rock outcrop and ~30% other soils (Soil Survey Staff, 2008).

2.2. Sample collection

A total of 426 soil samples were collected both horizontally on the surface and vertically on soil profiles in three soil samplings in Louisiana. The first group was composed of 55 surface soil samples collected from the Iberia Research Station, Louisiana State University Agricultural Center, Iberia Parish, which is mainly used as pasture for cattle, covers an area of ~202 ha, and consists of three soil map units, i.e., Gallion–Perry complex (Ga), Baldwin silty clay loam (Ba), and Iberia silty clay (Ib). The second group included 288 soil samples collected in 72 soil profiles at 10 cm increments to 40 cm depths from the three soil series in St. Landry Parish, i.e., Gallion, Latanier, and Sharkey soil series, of which 24 profiles each were from three land use types, i.e., cropland, wetland reserve program (WRP), and natural forest. The third group consisted of 83 soil samples from horizons of 12 soil pedons with coverage of forest and cropland, scattered across four parishes (East Feliciana, Rapides, St. Landry, and Iberville). These samples were associated with 12 soil series (Betis-R1, Cancienne-I3, Commerce-I1, Fluker-E1, Gallion-S1, Latanier-S2, Norwood-R3, Patoutville-S4, Ruston-R2, Schriever-I2, Sharkey-S3, and Tangi-E2) (Fig. 1a, Table 1), of which six pedons (R1, R2, R3, S1, S2, and S3) were sampled at 10 cm depth increments to 100 cm and the others were sampled on morphologically described horizons. The coordinates of these points were recorded by a handheld e-Trex (Garmin, Olathe, KS, USA) global positioning system (GPS) unit.

Capulin Volcano National Monument was divided into a grid of equilateral triangles; each with an area of ~3.75 ha. The triangle sampling scheme was expected to give slightly more precise estimates than the same effort on a grid of squares (McBratney and Webster, 1983). Within each triangle, three points were randomly selected, and sequentially a geometric center of the three selected points was calculated for further interpolation. The coordinates of these points were then uploaded into a handheld Garmin e-Trex GPS unit. Surface soil samples (0–12 cm) of equal quantities were collected from each point according to the guidance of the GPS unit. The three subsamples from each triangle were composited into one bag for further analysis. Eventually, 134 composited surface samples were collected from the surface of the Monument and 18 samples were collected from the horizons of the five pedons (C1–C5) described on the Monument (Fig. 1b). Additionally, six surface soil samples (0–12 cm) were collected for comparison at two nearby volcanoes: Mud Hill and Horseshoe (Fig. 1b). The entire Monument and nearby volcanoes were covered by naturally developed local vegetation such as pinyon trees, juniper trees, grasses, and miscellaneous shrubbery.