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Three-dimensional mapping of soil chemical characteristics at micrometric scale: Statistical prediction by combining 2D SEM-EDX data and 3D X-ray computed micro-tomographic images

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Many soil properties and functions emerge from interactions of physical, chemical and biological processes at microscopic scales, which can be understood only by integrating techniques that traditionally are developed within separate disciplines. While recent advances in imaging techniques, such as X-ray computed tomography (X-ray CT), offer the possibility to reconstruct the 3D physical structure at fine resolutions, for the distribution of chemicals in soil, existing methods, based on scanning electron microscope (SEM) and energy dispersive X-ray detection (EDX), allow for characterization of the chemical composition only on 2D surfaces. At present, direct 3D measurement techniques are still lacking, sequential sectioning of soils, followed by 2D mapping of chemical elements and interpolation to 3D, being an alternative which is explored in this study. Specifically, we develop an integrated experimental and theoretical framework which combines 3D X-ray CT imaging technique with 2D SEM-EDX and use spatial statistics methods to map the chemical composition of soil in 3D. The procedure involves three stages 1) scanning a resin impregnated soil cube by X-ray CT, followed by precision cutting to produce parallel thin slices, the surfaces of which are scanned by SEM-EDX, 2) alignment of the 2D chemical maps within the internal 3D structure of the soil cube, and 3) development, of spatial statistics methods to predict the chemical composition of 3D soil based on the observed 2D chemical and 3D physical data. Specifically, three statistical models consisting of a regression tree, a regression tree kriging and cokriging model were used to predict the 3D spatial distribution of carbon, silicon, iron and oxygen in soil, these chemical elements showing a good spatial agreement between the X-ray grayscale intensities and the corresponding 2D SEM-EDX data. Due to the spatial correlation between the physical and chemical data, the regression-tree model showed a great potential in predicting chemical composition in particular for iron, which is generally sparsely distributed in soil. For carbon, silicon and oxygen, which are more densely distributed, the additional kriging of the regression tree residuals improved significantly the prediction, whereas prediction based on co-kriging was less consistent across replicates, underperforming regression-tree kriging. The present study shows a great potential in integrating geo-statistical methods with imaging techniques to unveil the 3D chemical structure of soil at very fine scales, the framework being suitable to be further applied to other types of imaging data such as images of biological thin sections for characterization of microbial distribution.

Key words: X-ray CT, SEM-EDX, segmentation techniques, spatial correlation, 3D soil images, 2D chemical maps.