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Combining mid infrared and total X-ray fluorescence spectroscopy for prediction of soil properties

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Mid-infrared diffuse reflectance spectroscopy (MIR) can predict many soil properties but extractable nutrients are often predicted poorly. We evaluated the potential of MIR and total elemental analysis using total X-ray fluorescence spectroscopy (TXRF), both individually and combined, to predict results of conventional soil tests. Total multi-elemental analysis provides a fingerprint of soil mineralogy and could predict some soil properties and help improve MIR predictions. A set of 700 georeferenced soil samples associated with the Africa Soil Information Service (AfSIS) (www.africasoils.net) from 44 stratified randomly-located 100-km^2 sentinel sites distributed across sub-Saharan Africa were analysed for physico-chemical composition using conventional reference methods, and compared to MIR and TXRF spectra using the Random Forests regression algorithm and an internal out-of-bag validation. MIR spectra resulted in good prediction models (R^2 >0.80) for organic C and total N, Mehlich-3 Ca and Al, and pH. To test the combined spectroscopic approach, TXRF element concentration data was included as a property predictor along with the first derivative of MIR spectral data using the RF algorithm. Including TXRF did not improve prediction of these properties. TXRF was poorer (R^2 <= 0.68) in predicting organic C, total N compared to MIR (R^2 > 0.86) as these elements are not directly determined with TXRF, however the variance explained is still quite high and may be attributable to TXRF signatures relating to mineralogy correlated with protection of soil organic matter. TXRF model for Mehlich-3 Al had excellent prediction capability explaining 81% of the observed variation in extractable Al content and was comparable to that of MIR (R^2 = 0.86). However, models for pH and Mehlich-3 exchangeable Ca exhibited R^2 values of 0.74 and 0.79 respectively and thus had moderate predictive accuracy, compared to MIR alone with R^2 values of 0.82 and 0.84 respectively. Both MIR and TXRF methods predicted soil properties that relate to nutrient buffering capacity, including some exchangeable bases, pH, and organic matter content, and fingerprint basic soil mineralogy. Further work should investigate whether MIR and TXRF fingerprinting could better predict soil nutrient supply capacity, as determined by crop nutrient uptake, than conventional soil tests.