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How do different particle sizes affect mid infrared spectra and their spectroscopic calibrations?

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Soil analysis by mid-infrared (mid-IR) diffuse reflectance spectroscopy provides rapid and accurate estimates of soil properties. Although the method is rapid, sample preparation is time consuming. In fact soil samples are commonly ground to a fine particle size of around 250μm due to the 1 or 2 mm beam aperture of the spectrometers. Large particles can generate specular reflectance which dominates the DRIFT spectrum, thus grinding to 250μm enables to get more diffuse reflectance signals. Here we perform experiments to investigate the effect of different particle sizes on mid-IR diffuse reflectance spectra. The aims of this paper are to: (i) compare different particle sizes (2000μm, 1000μm, 500μm, 250μm and 106μm) on the frequencies of the mid-IR spectra, and (ii) compare the effect different particle sizes on the accuracy of spectroscopic calibration to predict soil pH, carbon, clay, silt and sand. Two hundred and eighty four samples were selected from the CSIRO's National Soil Archive. We analysed their mid-IR spectra with a FT-IR spectrometer, the Vertex70 (Bruker, Germany). To achieve the different particle sizes, we ground the samples using an agate mortar and pestle. Three replicates were used in the experiments. For our first aim, we analysed the data using an analysis of variance, which compared the effects of grinding to different particle sizes on individual frequencies. Results show that the spectra from all particle sizes are more similar in the fingerprint region between 1400 and 600 cm-1. For our second aim, we used a Partial Least Square Regression (PLSR) to predict the soil properties. There were no significant differences in the calibrations for soil carbon using soil at 1000μm, 500μm, 250μm and 106μm particle sizes. For clay the best prediction was obtained with 106μm, for silt the best predictions are obtained with 1000μm and 500μm and for sand the best predictions with 250μm and 106μm. Total reflection can occurs due to quartz peak intensity and this phenomenon can mask other peaks. By grinding to fine particles this phenomenon can be reduced in favour of the reflectance signal, thus clay and sand contents can be better predicted. For pH similar predictions are obtained with 250μm, 500μm and 1000μm. Grinding the samples to very fine particle sizes does not always increase the accuracy of mid-IR analysis and can have opposite effects for some properties, the analysis on particle sizes larger than 250μm can save time without losing the accuracy of mid-IR information.