



The potential of mid-infrared spectroscopy for the determination of soil physical, chemical, and biochemical properties on undisturbed soil samples

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Diffuse reflectance infrared Fourier transform (DRIFT) spectroscopy in the mid-infrared range has become an established analytical tool for qualitative and quantitative analysis of soils. The heterogeneity of soils requires sample preparation procedures to optimize the reproducibility and accuracy of spectroscopic measurements. Generally, soil is dried and ground before spectral measurement to avoid reflections of surface water films and minimize the intra- and inter-particle variability. However, these sample preparation techniques are limited to disturbed samples. The aim of this study is to evaluate the potential of DRIFT-spectra to determine soil properties on undisturbed soil samples. As approximation for undisturbed soil samples, in a first step, sieved soil samples were used and their spectral information were qualitatively compared with ground soil samples.

For this study, we used a pool of 240 soil samples originating from different sites across North Rhine-Westphalia (Germany) and West Africa. Samples covered a wide range of chemical, physical, and biological soil parameters. Soils were air-dried after sampling, sieved to <2 mm, and analyzed for SOC content, texture, iron oxides, CEC and pH-values. The DRIFT spectra of each sample were obtained in the laboratory using a Bruker Tensor27 benchtop FTIR equipped with an automated HTS-XT microplate reader. To compare MIR spectra of undisturbed and disturbed soil samples, sieved as well as finely ground soil samples were analyzed.

To focus on qualitative differences between the spectral subsets (sieved and ground), scattering effects had to be minimized, especially for the sieved-only sample set. Hence, spectra were offset corrected with the minimum value and the standard normal variate (SNV) was calculated for all spectra of both subsets for further processing. After pre-processing, both spectral datasets could be statistically separated in ground and sieved-only spectra using principal component analysis. Thus, the grinding procedure altered the spectral information. It is likely that the grinding process broke up soil aggregates and altered the surface structure of the soil samples, especially clay minerals as well as Fe-oxides seem to be masked by organic matter coatings. Correlation analysis between ground and sieved only spectral datasets showed spectral differences especially in the spectral regions around 1613 cm⁻¹ (structural water in clay), 1300 – 1150 cm⁻¹ (Si and Ca containing minerals), around 1116 cm⁻¹ (Al-Si in clay), and around 800 cm⁻¹ (quartz). To analyze the qualitative differences between the two subsets in more detail, similar spectra of the ground dataset were grouped using the k-means cluster algorithm. As a result, spectra were separated into three clusters varying especially in Fe-oxide as well as clay content. Within these clusters differences between the subsets sieved-only and ground have been analyzed using correlation analyses and the student t-test. For a profound interpretation of the significant spectral differences between these datasets, samples with the greatest spectral differences between sieved-only and ground were visually and chemically analyzed by SEM-implementation. In a next step, partial least square algorithm will be used to predict soil properties based on spectral information gained from sieved-only soil samples.