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Effects of the geometry of soil surface structures on DRIFT Spectra – Beam Trace Modelling and measurements

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The Fourier transformed infrared spectroscopy in diffuse reflectance mode (DRIFT) could be a useful for the in situ characterization of soil organic matter (SOM) composition at structural surfaces of preferential flow paths, such as fissures, soil aggregates and biopores. However, since such surfaces are mostly not plane, DRIFT requires a consideration of effects of local-scale surface geometry or structure on the signal. The geometrical effects on infrared (IR) signal intensity, such as particle size, porosity, pore size and shape, and relief exposition are known in principle, however, not well enough for quantifying its influence on the signal.
Our objectives are to measure and to model the influences of (i) the particle size, (ii) the porositiy, and (iii) specific surface shapes on the IR signal intensity. The comparison of the results shall disclose whether both approaches comes to the same conclusion and thus underpin each other. DRIFT measurements are carried out using coarse-textured quartz particle samples and gypsum blocks with defined surface shapes (i.e., pores, channels, ridges). A beam trace model (BTM) is used for the physical description.
The results show that the proportion of primary reflection increases for larger particle sizes so that their specular properties need to be considered separately. The application of the Kubelka-Munk transformation, which was developed for finely-ground samples, is found to be limited when studying the SOM composition of intact soil aggregate surfaces; here locally differing porosities and unevenness of the aggregate surface affect the reflection intensities. Results from measurements and modelling are in good accordance. Thus, the usage of a radiative transfer model might be a suitable approach for the interpretation of DRIFT signals.