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Spatial distribution of particulate organic matter pools, quantified and characterized by mid-infrared spectroscopy

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Comprising more than 60 % of the terrestrial carbon pool, soil organic carbon (SOC) is one of the principal factors regulating the global C–cycle. Against the background of worldwide increasing CO2 emissions, much effort has been put to the modelling of soil–C turnover in order to evaluate its potential for mitigation of climate change. Soil organic matter is an ever changing assemblage of various organic components that interact with the mineral matrix and in dependence of its ecological environment. Carbon storage is thereby assumed to propagate by hierarchical saturation of different carbon pools. A homogeneous distribution of the respective pools within natural environments is unlikely as the controlling soil parameters are subject to spatial and temporal heterogeneity. Several attempts to operationalize this complex soil compartment have been proposed, most of them resting upon a concept of pools with different stability and varying turnover times. Among these pools, particulate organic matter (POM) is considered to be most sensitive to environmental changes and has been shown to explain major parts of the SOC variations.

Until today, rather laborious physical and physico–chemical fractionation procedures are most commonly applied for the initialization and validation of POM in C–turnover models. Mid–infrared spectroscopy (MIRS) in combination with partial least squares regression (PLSR) could overcome this problem. The technique is fast, cheap, and requires little sample preparation. All the same, it is an appropriate technique not only for the determination of gross parameters like total soil organic carbon contents, but also for the determination and characterization of minor constituents like black carbon in soils. Basically, the infrared radiation is absorbed by molecules that express a dipole–moment during vibration. As virtually all constituents of soil organic matter and also a multitude of inorganic soil constituents express such a dipole–moment, plentiful chemical information can be extracted from absorption spectra of soil samples. In this work we present the development of calibration models for POM quantification via MIRS–PLSR, and the compilation of a raster data set including SOC and POM of three size classes for the testsite of the SFB–TR32 at Selhausen near Jülich (Germany).

The studied test site is an orthic luvisol which has been sampled in a ten times ten meter raster from 0–30 cm depth (n=131). For POM fractionation samples were gently sonicated and material from 2000–250 μm was gained by wet sieving. After a second, more intense sonication, intermediate (250–53 μm) and fine (53–20 μm) material was also gained by wet sieving. All fractions were dried at 40 °C, carbon contents were determined by elemental analysis.

For calibration of MIRS–PLSR, SOC contents of 87 bulk soil samples were determined by elemental analysis. Contributions of the different POM fractions to bulk SOC as well as the SOC contents within the particular POM fraction were determined for 36 soil samples by physical particle size fractionation as described above. MIRS-PLSR based predictions for the contribution of POM fractions to bulk soil proved to be satisfactory (R^2 >0.77) and improved with decreasing particle size. For the predictions of SOC contents in bulk soil and the different POM fractions R^2 even reached values $\geq$0.97. Root mean squared errors of the cross validations were in the range of standard deviations of the lab analysis or smaller. As physical fractionation methods are intrinsically susceptible to measurement errors, determination of POM fractions by MIRS analysis may even improve data sets for modelling. Apart from the generally convincing statistical parameters, further evidence for reliable predictions of the contributions of the different POM fractions to bulk SOC could be drawn from the spectral information itself. The spectral features utilized for the determination of the contribution of the different POM fractions to bulk SOC were matching the features for the prediction of the absolute SOC concentrations within the particular fractions. As these predictions were conducted with independent sample sets (bulk soil for the POM contribution and soil fractions for the SOC content within the fraction) the matching structural information for both features of the individual POM fraction indirectly validates the prediction for the POM pools. The latter is especially true as the observed features coincide with the actual knowledge on chemistry and stabilization of POM in soils.

For the compilation of a complete raster data–set, the developed calibrations were applied to all of the 131 topsoil samples taken at the SFB–TR32 testsite. Correlation analysis indicated that the coarse and the intermediate POM fractions are related to each other, to bulk SOC content and textural parameters respectively, while the fine POM fraction seems to be independent from these factors. The observed coherences and the applicability of a C–saturation concept will be discussed by visual map–comparison and geostatistical analysis of the determined parameters.