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Prediction of labile carbon pools in soil using near and middle infrared spectroscopy

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Rapid estimation of the amount and stability of soil organic carbon (SOC) by infrared spectroscopy has been proposed as a means to inform land use decision-making for the optimization of environmental services provided by soils. Our research tests the viability of this strategy by determining the accuracy and robustness of models predicting total and labile SOC content using near (NIRS) and middle (MIRS) infrared spectroscopy. Soil samples were collected from the 0-20 cm depth of arable fields in Germany with variable texture and SOC contents. Seven treatments were applied to 20 soils, including application of 2, 4 or 8 g C per kg soil in the form of straw or clover residues, as well as a control treatment without residues. Samples were then incubated for 56 days at 20˚C and cumulative CO_2 emissions were determined. Additionally, SOC, total nitrogen (N_t), NIRS and MIRS were measured on dried, milled samples before and after incubation, as well as microbial biomass (C_{mic}) after incubation. Partial least square regression (PLSR) and support vector machine regression, both with and without mathematical pretreatments, were compared as a means to estimate SOC, N_t, C_{mic} and labile C, quantified as the residue application rate, cumulative CO_2 loss during incubation, or the difference in bulk SOC before and after incubation. Separate models for straw and clover were created, both calibrated and cross-validated using control and 8 g C kg^{-1} soil residue treatments (n=40), and validated using 2 and 4 g C kg^{-1} soil residue treatments (n=40). While PLSR validation estimations of bulk SOC and N_t by both MIRS and NIRS can be categorized as good to excellent according to the ratio of performance to interquartile distance, estimations of labile C ranged from not usable to approximately quantitative. Neither spectral region consistently outperformed the other, suggesting there is value in utilizing both NIRS and MIRS when possible. As a measure of model robustness, models calibrated with samples prior to incubation were also used to predict SOC and Nt after incubation, when substantially less labile SOC was present. Compared to mathematically pretreated models optimized in cross-validation, models using untreated data for all wavelengths were a more robust means to accurately predict total SOC and N_t when the amount of labile C differed greatly from the calibration dataset.