Geophysical Research Abstracts
Vol. 16, EGU2014-3836, 2014
EGU General Assembly 2014

Mid-infrared spectroscopy as a tool to identify and quantify soil organic carbon size fractions

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Models such as CENTURY or RothC have been developed to simulate the dynamics of soil organic carbon. These models are very sensitive to errors in initial conditions and recent studies have identified the distribution of organic matter over the different pools as one of the largest sources of uncertainty. Each modeled carbon pool is characterized by a specific turnover rate that is linked to particular stabilization mechanism of organic matter. Different mechanisms of stabilization exist: physical protection, chemical and biochemical stabilization. Empirical studies have shown that these mechanisms can be, in part, functionally related to size fractions because some properties of soil organic matter such as its composition or dynamics depend on its size. Hence, information on carbon pool distribution could potentially reduce uncertainties associated with model simulations. However, current soil carbon fractionation schemes are costly and time-consuming.

Here, we investigated if mid infrared spectroscopy can be used to more quickly characterize these fractions. We analyzed soil samples from four long term trials in the USA under different tillage practices (no-tillage, conventional tillage or native sod) at two depths (0-5 cm and 5-20 cm) and on different soil types (Mollisol, Alfisol, Ultisol). Seventy samples, fractionated following Six et al. (2000) to identify functional C pools (> 2 mm, 2000-250 μm, 250-53 μm and <53μm) were used. The mid-infrared spectra of 350 samples (4 fractions plus bulk soil) were recorded with a FT-IR spectrometer.

The mean spectrum by size fraction shows significant spectral variations that are produced by aliphatic and aromatic organic groups as well as polysaccharides.

Each size fraction can be characterized by the spectral features generated by these groups.

After identifying the wavenumbers ranges linked to these groups, multivariate calibration models are built by using, as variables, only the absorbance calculated in these parts of spectra to quantify organic carbon in each fraction.

By preselecting variables, we are able to improve the performance of the models to predict C content in size fractions compare to a traditional PLS regression applied on the entire spectra in particular for the fine fraction (<53μm).

Using a traditional PLS regression, we observed a RMSE of 1.21 gC/kg and a RPD < 2. In contrast, using the functional groups as described above we are able to model the C content in the fine fraction with a RMSE=1.1 gC/kg and RPD=2.35.

We conclude that this new approach to quantify C content in size fraction represents an enhancement in the understanding of the functional organic groups that play a role in the different size fractions.

Key words: mid infrared reflectance (MIR) spectroscopy, soil organic carbon, physical fractionation.