Geophysical Research Abstracts
Vol. 16, EGU2014-14043-2, 2014
EGU General Assembly 2014

Assessment of organic matter resistance to biodegradation in volcanic ash soils assisted by automated interpretation of infrared spectra from humic acid and whole soil samples by using partial least squares

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From a practical viewpoint, the most interesting possibilities of applying infrared (IR) spectroscopy to soil studies lie on processing IR spectra of whole soil (WS) samples [1] in order to forecast functional descriptors at high organizational levels of the soil system, such as soil C resilience.

Currently, there is a discussion on whether the resistance to biodegradation of soil organic matter (SOM) depends on its molecular composition or on environmental interactions between SOM and mineral components, such could be the case with physical encapsulation of particulate SOM or organo-mineral derivatives, e.g., those formed with amorphous oxides [2].

A set of about 200 dependent variables from WS and isolated, ash free, humic acids (HA) [3] was obtained in 30 volcanic ash soils from Tenerife Island (Spain). Soil biogeochemical properties such as SOM, allophane ($Al_o + 1/2\ Fe_o$), total mineralization coefficient (TMC) or aggregate stability were determined in WS. In addition, structural information on SOM was obtained from the isolated HA fractions by visible spectroscopy and analytical pyrolysis (Py-GC/MS).

Aiming to explore the potential of partial least squares regression (PLS) in forecasting soil dependent variables, exclusively using the information extracted from WS and HA IR spectral profiles, data were processed by using ParLeS [4] and Unscrambler programs.

Data pre-treatments should be carefully chosen: the most significant PLS models from IR spectra of HA were obtained after second derivative pre-treatment, which prevented effects of intrinsically broadband spectral profiles typical in macromolecular heterogeneous material such as HA. Conversely, when using IR spectra of WS, the best forecasting models were obtained using linear baseline correction and maximum normalization pre-treatment.

With WS spectra, the most successful prediction models were obtained for SOM, magnetite, allophane, aggregate stability, clay and total aromatic compounds, whereas the PLS-model for TMC was of little significance. On the other hand, the best successful prediction models using HA spectra were for SOM, TMC, allophane content and soil fungal pigments.

In these particular volcanic ash soils, with large concentration of short-range minerals, the use of WS spectra, compared to the use of HA spectra, led to predict higher number of dependent variables. This is interpreted as the fact that the information of mineral constituents may help to explain soil emergent properties (e.g., SOM resilience or hydrophysical properties).

The above results coincide with previous research [2] based on classification of soil properties by multidimensional scaling, where it was demonstrated that formation of stable organomineral complexes between HA and allophane coincide with large amounts of SOM and low TMC values.

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