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Assessing Soil Organic Matter Thermal Stability with i-Chemometrics

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Soil organic matter (SOM) thermal stability is associated with SOM quality and therefore with its fate along carbon and nitrogen cycles. Understanding the chemical aspects of SOM thermal stability is essential to predict soil adaptability to climate change, particularly the responses of SOC and SON pools. SOM thermal stability influences SOC residence times and the size of the SON pool; this is due to the association between thermal and biological stability and to the storage of N in thermally stable heterocyclic compounds.

However, providing a consistent measurement of SOM thermal stability is challenging. In spite of the availability of different analytical techniques (e.g. thermogravimetry (TG), differential scanning calorimetry (DSC)), and the enhanced resolution provided by complimentary spectroscopic analysis (e.g. FTIR, NMR), combining the outputs from this analysis into a single metric is complicated.

In this research, we explore the potential of i-Chemometrics to provide a comprehensive measurement of SOM thermal stability. i-Chemometrics stands for information theory based chemometric analysis. As many other chemometric techniques, i-Chemometrics is data driven and looks for hidden patterns in multivariate datasets, representing sample points in a reduced dimensional space. However, the information theory framework that supports it provide a unique advantage over other common approaches (e.g. Principal component analysis, Partial Least Squares): i-Chemometric dimensional spaces have specific geometric properties, i.e. they are invariant regardless the composition of the samples. These geometric properties allows for the identification of consistent metrics across highly heterogeneous sets of samples.

To illustrate the application of i-Chemometrics in the estimation of SOM thermal stability metrics we analyze U.S. soil samples covering a wide range in organic carbon concentration (13 to 243 gC kg-1), mineralogy and land use. Samples were analyzed using TG-DSC, and after heating to specific end-point temperatures, FTIR spectroscopy was used to analyze the molecular composition of each sample. We calculated the information entropy (i.e. Shannon's entropy) of FTIR spectra and used these values as inputs in the construction i-Chemometric spaces to map soil samples. Our results suggest that the location of the soils samples in i-Chemometric spaces could be used as a metric for soil thermal stability encompassing the effects of organo-mineral interactions as well as differences in initial organic carbon content.

Further research looks to expand the size of our original dataset and testing the influence of experimental conditions in the calculation of more accurate SOM thermal stability metrics. We think that our approach could be extended to other spectroscopic analysis (e.g. GC/MS, NMR), providing a simple, yet robust framework for the assessment of fundamental properties of soils that determine its quality and adaptability.