Geophysical Research Abstracts
Vol. 14, EGU2012-13957, 2012
EGU General Assembly 2012

Dissolved organic carbon (DOC) in soil extracts investigated by FT-ICR-MS

D. Hofmann (1), D. Steffen (2), N.D. Jablonowski (3), and P. Burauel (1)

(1) Agrosphere Institute (IBG-3) , Forschungszentrum Jülich GmbH , (2) Jülich Supercomputing Centre (JSC), Forschungszentrum Jülich GmbH, (3) Institute of Bio- and Geosciences, IBG-2: Plant Sciences, Forschungszentrum Jülich GmbH

Soil drying and rewetting usually increases the release of xenobiotics like pesticides present in agricultural soils. Besides the effect on the release of two aged 14C-labeled pesticide residues we focus on the characterisation of simultaneously remobilized dissolved organic carbon (DOC) to gain new insights into structure and stability aspects of soil organic carbon fractions. The test soil (gleyic cambisol; Corg 1.2%, pH 7.2) was obtained from the upper soil layer of two individual outdoor lysimeter studies containing either environmentally long-term aged 14C residues of the herbicide ethidimuron (0-10 cm depth; time of aging: 9 years) or methabenzthiazuron (0-30 cm depth; time of aging: 17 years).

Soil samples (10 g dry soil equivalents) were (A=dry/wet) previously dried (45°C) or (B=wet/wet) directly mixed with pure water (1+2, w:w), shaken (150 rpm, 1 h), and centrifuged (2000 g). This extraction procedure was repeated several individual times, for both setups. The first three individual extractions, respectively were used for further investigations. Salt was removed from samples prior analysis because of a possible quench effect in the electrospray (ESI) source by solid phase extraction (SPE) with Chromabond C18 Hydra-cartridges (Macherey-Nagel) and methanol as backextraction solvent.

The so preconcentrated and desalted samples were introduced by flow injection analysis (FIA) in a fourier transform ion cyclotron resonance mass spectrometer (FT-ICR-MS), equipped with an ESI source and a 7 T supra-conducting magnet (LTQ-FT Ultra, ThermoFisher Scientific).

This technique is the key technique for complex natural systems attributed by their outstanding mass resolution (used 400.000 at m/z 400 Da) and mass accuracy ($\leq$ 1ppm) by simultaneously providing molecular level details of thousands of compounds and was successful applied for the investigations of natural organic matter (NOM) different sources like marine and surface water, soil, sediment, bog and crude oil.

The characteristics of measured DOM mass spectra were demonstrated. Furthermore, an algorithm to compute all chemically relevant C,H,O-, C,H,(O,S),N- as well as C,H,(O),S molecular compositions, designed and exercised by ourself using Scilab routines, was used for entire structure elucidation.

Various methods for data evaluation of such an amount of peaks are applied to describe the characteristics of DOC. The van Krevelen diagram is widely used to classify the DOC compounds regarding polarity and aromaticity, whereas the Kendrick diagram allow to identify ions with elemental formulas that differ only in CH2, and molecular formulas with similar Kendrick Mass Defect (KMD) can be sorted by nominal mass series. Both kind of diagrams were developed and results are discussed together with the findings of ETD, MBT, and metabolites after soil drying and rewetting. Overall, the results suggest that intermittent soil drying and rewetting alters the disaggregation of soil aggregates, resulting in a release of entrapped organic carbon as well as pesticide molecules.