



UFZ-Seminar „Water and Environment“

18 September, 3 pm

Seminar Room 1, Brückstr. 3a, Magdeburg or

<https://ufz-de.zoom.us/j/6831992537?pwd=VXZFSmF3ZDZ3ckJ0dEUxNUQzSHR6QT09>

Carsten Simon

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will give a talk on

Parallel analysis of dissolved and particle-associated organic matter fractions via ultrahigh resolution mass spectrometry

Organic matter (OM) is an important component of soils and sediments that contributes to manifold aspects of their reactivity, metabolic activity and environmental behaviour (e.g., retention or release of C or nutrients). The molecular structure of OM, however, remains largely elusive. Ultrahigh resolution mass spectrometry (like FT-ICR-MS) has contributed new impulses to the study of molecular properties of the soluble fraction of OM, i.e., dissolved organic matter (DOM) via electrospray ionization (ESI), but remains “blind” to the much larger non-soluble fractions of OM. Traditionally, this problem was tackled by employing more potent solvents, such as alkaline extractants. Recently, alternative ionization sources such as laser desorption ionization (LDI) have shown promising results to extend the analytical window of FT-ICR-MS and to achieve a more complete insight into OM chemistry through direct analysis of particle surfaces. In this context, we here discuss outcomes of LDI analyses of OM fractions based on two datasets: 1) arable topsoils (2-20cm depth) from four long-term experiments (Dikopshof, GER, U Bonn, since 1940; Reckenholz, CH, Agroscope, since 1949; Thyrow, GER, HU Berlin, since 1937; and Orgeval, FRA, INRAe, since 1998) under no fertilization and farmyard manure fertilization regimes, and 2) sequential extractions of sedimentary OM from the Rappbode predam reservoir. For dataset 1), direct analysis of particles was conducted and compared to aqueous DOM extracts considering molecular trends in e.g., aromaticity or nominal oxidation state, with the aim to understand molecular differences in stabilized OM between treatments and their duration. For dataset 2), molecular trends obtained from remaining particle-associated OM after each extraction step were put in context of existing radiocarbon data to obtain better understanding of sedimentary organic matter composition and stabilization mechanisms. Results from both datasets will be discussed in the light of recent views on molecular mechanisms behind OM stabilization in the environment. Together, our results suggest that direct analysis of soil and sedimentary particles is a fast, reproducible, sensitive and less labor-intensive alternative to routine DOM analyses employing ultrahigh resolution mass spectrometric detection, with various potential applications (e.g., for samples that yield only low amounts of DOM, or where only small amounts of sample are available). However, for a maximum molecular insight, and due to systematic differences in analytical windows of ESI and LDI, a combination of both ionization methods is still recommended.