Thermal Analysis High-Resolution Mass Spectrometry for Molecular Insights into Complex Soil Organic Matter

Christopher P. Rüger[1,2], Eric Schneider[1,2], Anika Neumann[1,2], Lukas Friederici[1,2], Vera Samburova[3], Hendryk Czech[1], Ralf Zimmermann[1,2]

1 – University of Rostock, Chair of Analytical Chemistry, Joint Mass Spectrometry Centre (JMSC), 18059 Rostock, Germany

2 – University of Rostock, Department Life, Light & Matter (LL&M), 18059 Rostock, Germany

3 – Division of Atmospheric Sciences, Desert Research Institute, Reno, NV 89512, USA

It is well known that wildfires affect flora and fauna, burn various fuels, and emit large quantities of gases (*e.g.*, CO_2 and CO) and particles (*e.g.*, black, brown, and organic carbon) that are further modified during atmospheric transport. Wildfires significantly affect air quality, human health, cloud formation and properties, and atmospheric light absorption and radiative forcing in the atmosphere and after deposition onto snow. Moreover, wildfires also alter soil properties, including soil wettability (or water repellency). Fire-induced soil water repellency (SWR) decreases water infiltration, leading to increased runoff, soil erosion, flooding, and debris flows.

Despite a significant effort and several comprehensive studies on the chemistry of post-fire organic constituents in soils, a large gap remains in the current knowledge and understanding of which organic compounds are responsible for post-fire SWR. This study attempts to shed more light on the chemical nature of fire-induced SWR, using thermogravimetry (TG) atmospheric pressure photoionization (APPI) in combination with Fourier transform ion cyclotron resonance (FT-ICR) mass spectrometry (MS) (or TG APPI FT-ICR MS). The TG APPI FT-ICR MS method is a comprehensive state-of-the-art method to characterize complex mixtures of organic molecules, including organic constituents in soils.

The positive correlation between water repellency measures and aromaticity, derived from the APPI FT-ICR MS spectra for the desorption (or pre-pyrolysis) phase (~20–270 °C temperature range), suggests that burned soils may become water repellent because of the formation and/or deposition of PAH-like organic species on the soil surface. Moreover, we found that organic molecules with a higher amount of oxygen in their structure are more common in unburned than in burned soil samples, which may also have contributed to the more hydrophobic (or more water-repellent) behavior of the burned compared to the unburned soils.

References

Samburova, V.; Schneider, E.; Rüger, C.P.; Inouye, S.; Sion, B.; Axelrod, K.; Bahdanovich, P.; Friederici, L.; Raeofy, Y.; Berli, M.; et al. Modification of Soil Hydroscopic and Chemical Properties Caused by Four Recent California, USA Megafires. *Fire* **2023**, *6*, 186, doi:10.3390/fire6050186.

Rüger, C.P.; Miersch, T.; Schwemer, T.; Sklorz, M.; Zimmermann, R. Hyphenation of Thermal Analysis to Ultrahigh-Resolution Mass Spectrometry (Fourier Transform Ion Cyclotron Resonance Mass Spectrometry) Using Atmospheric Pressure Chemical Ionization For Studying Composition and Thermal Degradation of Complex Materials. *Anal. Chem.* **2015**, *87*, 6493–6499, doi:10.1021/acs.analchem.5b00785.