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Probing and modelling the surface reactivity of pyrogenic carbon

DANIEL S. ALESSI[1], KATHERINE N. SNIHUR[1], LINGYI TANG[1], DWI CANDRA PRATIWI[1], YUGE BAI[1], LOGAN R. SWAREN[1], JANICE P. L. KENNEY[2] AND KURT O. KONHAUSER[1]

[1]University of Alberta
[2]MacEwan University
Presenting Author: alessi@ualberta.ca

Pyrogenic carbon (PyC) is generated through natural wildfires and as a product of the commercial pyrolysis of biomass to produce charcoal for soil amendment and water treatment purposes. A crucial aspect in determining the efficacy of PyC in removing specific molecules or elements from water is developing a comprehensive understanding of its surface chemistry and reactivity. While many such studies rely on empirical adsorption models that have limited predictive capabilities under specific experimental conditions, surface complexation modelling (SCM) presents a promising alternative. SCM, grounded in equilibrium thermodynamics, inherently considers various factors influencing adsorption, such as solution pH, solution chemistry, and temperature. By integrating these factors into the modelling process, SCM offers a predictive framework that can adapt to changes in environmental conditions over time or location. For example, this approach can aid in the development of PyC that functions more effectively and sustainably in water treatment and sanitation strategies, or allows for a better understanding of the reactivity of wildfire-generated PyC towards nutrients and metals in soils, rivers and marine settings. This presentation will delve into several endeavors of applying SCM to PyC-containing systems, including the treatment of potentially harmful trace metals (e.g., Ni, Zn, U, Cr), the regulation of metals and nutrients in agricultural soils (e.g., Cd, Se), and the role of nanosized PyC in elemental transport. Additionally, a perspective on the future research required for the widespread application of the SCM approach to PyC in complex environments will be discussed.