Presentation Title: PFOS Sorption in Soils and the Prediction of Associated Sorption Coefficients by Machine Learning

Description: The influence of soil properties on the sorption of per- and polyfluoroalkyl substances (PFAS) using a wide range of temperate and tropical soils is not fully understood. Previous investigations utilised few soils ($n < 10$), particularly temperate soils, for the investigation of PFAS sorption behaviour in soils. In this study, we investigated PFOS sorption using 114 tropical and temperate soils that were collected from Australia and Fiji. Sorption isotherms were nonlinear. The equilibrium soil-water distribution coefficients (K_d) of PFOS varied in soils and were dependent on some key soil properties that include, total organic carbon content, anion exchange capacity, amorphous aluminium, and iron oxide contents, as well as pH and silt contents. We developed two artificial neural networks (ANN) for the prediction ($R^2 = 0.80$) of K_d in soils using the key soils properties, with the ANN models showing a 60% improvement over the K_d predictions by multiple linear regression. The ANN models were exported and deployed as a web application for hands-on prediction of PFOS K_d in soils. This study show that not only is the TOC content of soils important in describing PFOS sorption, but that the surface charge characteristics of soils are important as well. This study also presents the first application of machine learning for the prediction of PFOS sorption in soils.

Presenter's details

Brief biodata: Anthony Umeh completed his PhD in Environmental Remediation at the University of Newcastle in 2019 and he is currently a research associate at the University's Global Centre for Environmental Remediation. He has been working on the bioaccessibility and bioavailability of polycyclic aromatic hydrocarbons (PAHs) in soils since 2013, following his MSc at Lancaster University United Kingdom. His PhD thesis investigated the potential risks to human and ecological health from exposure to highly sequestered PAHs in long-term contaminated soils, using solvent extractions, *in vitro* bioaccessibility assays that simulates the human gastrointestinal system, and earthworm bioassays. Anthony's postdoctoral research focuses on understanding the fate and transport of PFAS in soils, as well as developing innovative remediation techniques for PFAS-contaminated soils and wastewater. His recent paper in Environmental Science & Technology presents the first application of machine learning for the prediction of PFOS sorption in a wide range of well-characterised tropical and temperate soils.