PhD project: Hugo de Campos Pereira

Sorption of perfluoroalkyl substances in soils – mechanisms and modelling

The main purpose of my PhD project is to substantially expand our knowledge on how poly- and perfluroalkyl substances (PFASs) bind to soil components on a molecular scale, and to use this knowledge to develop a general geochemical model with the capacity to predict the partitioning and speciation of PFASs in soils of diverse properties. The development of such a model is essential for improved environmental risk assessment of these chemicals, which today is severely limited by insufficient knowledge on how and to what extent PFASs are bound in soils.

Background

PFASs have been produced in large quantities since the 1960s for use in a wide range of industrial applications and consumer products. However, it was not until the late 1990s that the chemicals were recognized as contaminants of global concern as researchers then began to find PFASs ubiquitously distributed in the environment as well as in living organisms including humans. The chemicals are toxic to varying degrees, with one of the primary exposure routes for humans being drinking water. To better assess the environmental risks of PFASs, including the risk of leaching to raw water sources for drinking water production, a geochemical model with the ability to predict PFAS soil sorption and solubility would be a key tool.

Methods

Experimental methods of this doctoral project include batch experiments, ultra-performance liquid chromatography (UPLC), chemical soil extractions, and spectroscopic techniques such as neutron reflectrometry, extended X-ray absorption fine structure (EXAFS) spectroscopy and scanning transmission X-ray microscopy (STXM). In the model development, we will build on the existing modelling framework Visual MINTEQ (Gustafsson, 2013) and incorporate relevant binding mechanisms to organic and inorganic soil components into the Stockholm Humic Model (SHM) (Gustafsson, 2001) and the CD-MUSIC surface complexation model (Hiemstra and van Riemsdijk, 1996), respectively.