





## Sujet de thèse 2021 – ED chimie de Lyon

Prédiction du comportement à la lixiviation des matrices anthropiques à haute teneur en matière organique dans un scénario réel de valorisation

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Prediction of the leaching behaviour of anthropic matrixes highly charged in organic matter under natural exposure conditions in view of their valorization

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## Problematic and objectives

These past years, many initiatives have focused on developing nature-based solutions (NBS) for water and land management; in the field of urban drainage and domestic water management, such devices have even been preferred over conventional infrastructure, leading to a widespread use of, for example, treatment wetlands or stormwater basins. While purification/treatment performances of these systems were often largely investigated, the solid residues are often neglected. However, wastewater and stormwater also convey significant amounts of suspended solids (SS), which act as vectors for a series of urban- or traffic-derived substances. The accumulation of these SS at the surface of the installations leads to the formation of a residue with high organic content, which is variously referred to as sludge, organic deposit, anthropic matrixes or sediments depending on the context.

The management of these matrixes rises environmental aspects, which need to be considered. Anthropic matrixes contain nutrients of interest (e.g. N, P...), but are also charged in pollutants, notably trace metals (e.g. Zn, Cu, Ni, Cd, Co, Pb, Cr), which are susceptible of leaching to soil or groundwater, becoming a non-negligible threat towards aquatic and terrestrial organisms. On the other hand, these materials are highly charged in organic matter (humic and fulvic like), which plays an important role in the mobility and bioavailability of the metallic pollutants previously mentioned, by sorption and desorption mechanisms. Achieving a better understanding of the behaviour of these solid residues represents nowadays a major issue for their proper on-site and off-site management. After dredging, several valorisation paths have been already considered, such as agricultural application or valorisation in construction, but each solution faces difficulties and the possible environmental consequences of each practice have to be objectively outlined. The present thesis means at using geo-chemical modelling, coupled with transport and diffusion, in order to predict the leaching behaviour of these high organic anthropic matrixes exposed to natural conditions, in different scenarios.







## Methodology

Geochemical modelling has proved to be a useful tool in understanding and describing the leaching mechanisms of solid matrixes in complex systems. It has been currently used in the modelling of solid sludge deposit, in order to represent major and trace elements speciation and distribution of metallic pollutants between the solid and the liquid phase at thermodynamic equilibrium (*i.e.* without considering transport aspects). The fate of pollutants is influenced by the chemical parameter of the leachate (pH, Eh, ionic strength...) and by the different pure or carrier phases able to precipitate or dissolve and sorb pollutants. Organic matter is described as being composed of fulvic and humic acids with discrete specific sites distribution. The previously developed model considers three types of surfaces capable of sorbing metallic pollutants: particulate organic matter, soluble organic matter and particulate Fe oxides. The multisurface sorption Model VII and NICA-Donnan model, which use generic parameters to describe cation binding to humic substances, have been coupled with the geochemical calculation tool PHREEQC-v3, which uses the thermodynamic database LLNL.

However, the prediction of the leaching behaviour of solid matrixes exposed to natural conditions (dry and wet sequences, percolation, ...) cannot be achieved without including additional processes in the model. The most critical aspects to be considered are the transport and diffusion of metallic and organic compounds desorbed at the solid-liquid interface, within the porous matrix, and their potential interactions with deeper strata. For that purpose, the developed model at thermodynamic equilibrium will be coupled with a secondary modelling tool specialized in the modelling of soil hydrodynamics and transport phenomena, such as Hydrus or COMSOL Multiphysics. These modelling tools have been proven to accurately replicate water fluxes in a wide variety of homogenous and heterogeneous porous media; however, couplings with geochemical models to describe the fate of contaminants in complex matrixes such as those presented above still constitute an emerging field of research. Besides the physico-chemical characterisation of the studied matrix, percolation/column tests at pilot-scale will be used for the validation of the developed model.

## Context

DEEP laboratory has already built a strong expertise at international scale in the Nature-Based Solution investigation through several works and projects in the fields of stormwater management and treatment wetlands. Some collaborations will be established during this thesis. In the context of RESEED partnership, INRAE will be involved notably in the use of a model for transport investigation. Geoscience Rennes with their strong experience in geochemistry or LEHNA with their knowledge in porous media will also be involved in the current thesis.