## Multi-scale modeling of multiphase flows of complex fluids in porous media based on microfluidic experimentation and at the Darcy scale: application to the rehabilitation of polluted soils

Supervisors: Amine BEN-ABDELWAHED, Antonio RODRIGUEZ DE CASTRO

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## **General information**

Host laboratory: Institut de Mécanique et d'Ingénierie de Bordeaux (I2M) - porous media team.

*<u>Type of contract:</u>* 3 years PhD, full-time position. Gross salary: 2044-2300 € €/month.

Starting date: as soon as possible.

## Topic:

Water, food and energy form a nexus at the heart of sustainable development. The demand for all three is growing rapidly. Urban and agricultural environments are increasingly contaminated by chlorinated organic solvents, pesticides, nitrates, heavy metals, etc. These are added to the historical pollution resulting from our industrial heritage. These pollutants, which initially affect shallow soil layers, eventually seep into groundwater. Since groundwater is the largest reservoir of fresh water in the world, its quantity and quality are important for ecosystems and humans. Soil pollution also reduces the amount of land available for agriculture, as food and fodder crops absorb contaminants from the soil. This is not a trivial question given the current scarcity of agricultural land due to urban and industrial sprawl. It is therefore essential to restore degraded soils to resist current and future pressures and ensure water and food sovereignty. From an economic point of view, soil contamination could cost the EU up to 38 billion euros per year (source: European Commission). Unlike site rehabilitation processes by excavation, in situ treatments do not require ground movement and are less expensive.

However, in situ remediation requires the uniform delivery of treatment avoiding the appearance of preferential flow paths in the medium, which has proven to be a major obstacle to their full development. To remedy this, the injection of complex fluids is one of the few cost-effective strategies allowing in situ decontamination with minimal environmental impact. For example, polymers such as xanthan gum and polyacrylamide in its partially hydrolyzed form (HPAM) are generally added to aqueous solutions to increase the efficiency of macroscopic pollutant sweeping in polluted soil remediation operations. This better efficiency is obtained thanks to the optimization of the viscosity ratio between the injected and displaced fluids provided by these additives.

Knowledge of the physics of underground multiphase flows at the pore scale is therefore essential for designing effective soil remediation methods. Although significant progress in this field has recently been made by combining microfluidic experiments and numerical simulations, our knowledge of the dynamics of the immiscible displacements of pollutants remains very limited in the case where the displacing fluid is shear-thinning. Among the major obstacles are the requirements in terms of numerical resources necessary for the simulations of multiphase flows of non-Newtonian fluids in porous media and the difficulties inherent in the experimental measurement of viscosities and dynamic contact angles at the pore scale. This results in the scarcity of fundamental numerical work and experimental validation studies in the literature. Therefore, a multi-scale model is needed to study the influence that the shear rate-dependent dynamic viscosity exerts on the pollutant recovery rate, and this for different injection velocities and different wettability conditions.

To address this need, a series of microfluidic experiments (Figure 1) will be performed to identify microscopic mechanisms of displacement and quantify their impact on scanning efficiency. The detailed knowledge of the local mechanisms obtained thanks to microfluidics will make it possible to judiciously choose the controllable parameters (injection rate, formulation of the fluid) in a second series of 1D experiments which will be carried out using columns of sand and consolidated cores (Darcy scale). The effective properties at the Darcy scale, ie the residual saturation of the pollutant, the apparent viscosity of the shear-thinning fluid and the relative permeabilities will be quantified by measurements of gamma ray attenuation and pressure drop. Relationships between these effective properties and the process conditions will then be established. This experimental work will be completed by a numerical study allowing access to physical quantities that are difficult to measure, such as local viscosities. A schematic view of the envisaged approach is given in Figure 2.Les objectifs de cette thèse sont listés ci-dessous :

- Develop a multi-scale model to assess the efficiency and energy cost of an in situ remediation strategy based on soil properties (permeability, wettability, porosity, pore size distribution, connectivity), soil characteristics the shear-thinning fluid injected (formulation, rheology, surface tension) and the injection parameters (flow rate, pressure, sequencing of the injection steps).

- Identify the mechanisms and microscopic phenomena determining the quantity of pollutant trapped through advanced microfluidic experiments.

- Use these microfluidic experiments to characterize the distribution of dynamic contact angles in the porous medium, essential and unknown information for many environmental applications ranging from underground hydrogen storage to soil remediation.

- Implement a numerical code fed by the experimental results and allowing access to physical properties that are difficult to measure such as the distribution of viscosities and pressures in the medium.

- Validate the proposed model through experimentation at the core scale and quantification of the effective properties by gamma ray attenuation measurements (residual saturation) and pressure drop measurements.



**Figure 1.** Microfluidic setup similar to that which will be used in the planned experiments. A fluid is injected using a pump (syringe pump or imposed pressure pump) and the displacement of the fluid through the micromodel is recorded by a high-resolution camera coupled to an optical microscope.



Figure 2. Schematic view of the multi-scale modeling approach envisaged.

## **References**

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