Call for an outstanding PhD candidate working for an international collaborative project

Title of the project : Mechanics and transport in electrically charged porous media: homogenization using spectral methods. Application to nuclear waste storage.

BACKGROUND

Charged porous media such as concrete, clays, shales, soils, biological tissues are ubiquitous in almost all aspects of life. Penetration of chlorides ions through concrete leads to the depassivation of reinforcing bars and therefore may shorten the life of the structure. The electro-chemical mechanisms of water adsorption by smectites are of utmost importance in determining the ability of soils to transport and supply water. Clay swelling is of widespread relevance in geotechnical and geoenvironmental fields. Owing to the presence of binding agents for pollutants together with the low hydraulic conductivity, plastic character and self-sealing capacity, bentonitic clays have been suggested appropriate engineered barriers against environmental pollution to prevent the migration of pollutants. Electrokinetic phenomena near charged surfaces have other numerous technological applications such as in the remediation of contaminated soils, in the design of artificial membranes with high ion-exchange capacity, in filtration processes and in the development of efficient drug delivery substrates. The physiological states of soft connective tissues (articular cartilage and intervertebral disk) are partially swollen and exhibit prestresses which play an important role in the load bearing characteristics of articulating joints.

As such, it is imperative that any macroscopic model describing the complex electro-chemo-mechanical interaction inherent to this type of system contains the appropriate constitutive relations. Expansive materials have in common a structure that can be loosely identified as a three-scale materials. At the nanoscale (≈1 nm), the solvent is adsorbed in the form of an electrolyte solution with partially or totally dissociated ionic species. At the microscale (≈1 μm), the solvent also exists in bulk solution (free of any adsorptive force).

Since nearly ten years, the macroscopic model governing coupled electro-chemo-mechanical phenomena in charged porous media (swelling or not) has been revisited within a rigorous homogenization procedure applied to the microscopic governing equations which describe the local interaction between a charged solid phase and an aqueous electrolyte solution. The up-scaling of the microscopic electro-hydro-dynamics leads to a two-scale approach wherein the macroscopic model appears governed by a fully coupled form of Onsager's reciprocity relations, mass conservation equations and a modified Terzaghi's effective stress principle. This two-scale approach provides microscopic representations for the effective coefficients which are exploited to obtain further insight in the constitutive behavior of the electrochemical parameters and the swelling pressure. Among other effects, these microscopic closure relations are mainly dictated by the spatial variability of a microscale electric potential which satisfies a local version of the Poisson–Boltzmann problem in a periodic unit cell. This approach furnishes a precise definition at the macroscale of the mechanical properties of the materials (including the disjoining pressure), the diffusion coefficients (or tensors) for the ions, the permeability of the medium, the chemico-osmotic and electro-osmotic permeabilities.

These properties can be computed by solving a system of closure problems (partial derivative equations) on a unit cell. The computation is necessarily 3D to have both the solid phase and the pore phase connected and the cell geometry must be sufficiently complex to be representative of the porous material. This is therefore a cumbersome task. Some new spectral methods are now able to help the determination of the homogenized tensor without solving the complicated closure problems derived from the homogenization technique. They first appeared in the mechanical domain and began becoming efficient and popular in the early 2000s. They are now developed both for diffusive transport and flow transport through porous media. Some work is needed to adapt them to the up-scaling of ions transport through charged porous medium.

At the same time imaging techniques (IRM, MEB , FIB…) are growing up and are now able to furnish images at various scales of the porous material. Combining these imaging techniques with the spectral method to compute the homogenized coefficients (or tensors) will lead to multiscale model based on the experimental observation of real samples.

Finally, the consideration of chemical reactions in the modeling is also possible, through a coupling between the softwares Phreeqc and Comsol Multiphysics.

The aim of this PhD thesis is:

1. To understand the physics and to select the best modeling of the coupled transport phenomena through electrically charged porous materials at the smallest scale;
2. To perform the homogenization procedure depending on the retained physics at the considered scale;
3. To acquire images of the materials at the various scales (typically: FIB at the nanoscale; MEB at the microscale) in collaboration with BRGM Orléans;
4. To use spectral methods to compute step by step (from nano to micro; then from micro to macro) the effective coefficients of the constitutive equations at the macroscale.
5. To include chemical reactions in the modeling through a coupling between the softwares Phreeqc and Comsol Multiphysics.
6. To compare numerical results with experimental results.

TIMELINE

Year 1

- Literature study on coupled transport phenomena
- Reporting state-of-the art for introductory chapters of Ph.D. thesis.
- Acquiring ability to work with theoretical modelling of coupled transport phenomena in reactive porous materials

Year 2

- Thorough analyses of theoretical modelling of coupled transport phenomena in reactive porous materials
- Acquiring ability to work with the experimental facility with BRGM for image acquisition at the various scales (FIB at the nanoscale, MEB at the microscale)
- Acquiring ability to use spectral methods
- Presentation of results at a scientific conference (to be selected).

Year 3

- Careful experiments with the experimental facility at BRGM
- Thorough analyses to compute step by step (from nano to micro, then from micro to macro) the effective coefficients of the constitutive equations at the macroscale
- Including chemical reactions in the modeling through a coupling between the softwares Phreeqc and Comsol Multiphysics
- Comparison of numerical results with experimental results
- Publication of the results obtained in international journals
- Reporting results in chapters of Ph.D. thesis.

EMBEDDING AND FACILITIES

The PhD project will be executed within the framework of the international research group GdRI Multiphysics and Multiscale Couplings in Geomechanics. The GDRI GeoMech was created in January 2016, continuing the GDR MeGe. During 8 years, this GDR has gathered the main French groups involved in the broad field of geomechanics, with a special focus to environmental applications. Taking advantage of the different collaborations and connections that the partners had developed with foreign universities, extending the network in an international perspective was a natural ambition. The goal of the network (GDRI) is thus to gather and promote the French community involved in geomechanics, to strengthen its national and international visibility.
Currently, the GDRI GeoMech gathers more than 25 partners, coming from many countries including The Netherlands, Italy, Spain, Canada and China. Structuring the existing community working on Multi-Physics and Multiscale Couplings in Geo-environmental Mechanics, the main lines of research are:

- Catastrophic failures and triggering mechanisms
- Safety of storage reservoirs
- Energetic geomechanics.

Specifically, partners in the current project are:

- Dr. Olivier Millet, University of La Rochelle (France)
- Dr. Christian Moyne, University of Lorraine (France)
- Dr. Richard Wan, University of Calgary (Canada)
- Dr. Zhenyu Yin, Ecole Centrale de Nantes (France)
- Dr. Khaled Bourbatache, INSA de Rennes (France)

The PhD student will be stationed in France (at La Rochelle), will visit the French institutes for various periods and will benefit from the scientific workshops organized regularly by this international network. Indeed, the GDRI aims spreading and sharing up-to-date information about recent research on the subject, extending international collaborations as well as organizing international scientific meetings and other related events.
The project will be conducted in an open and collaborative environment, aimed at optimizing the advancement of science and the personal development of the PhD student.
Ultimately, the 3-year research will lead to a PhD thesis, to be defended at La Rochelle.

The student will benefit of the results already obtained by the proposers on the topic (see references below).

<u>**Collaboration /supervisor**</u>:

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STUDENT REQUIREMENTS

The student must have an M.Sc. degree in Civil, Mechanical or related Engineering discipline. As the project involves theoretical, experimental and simulation aspects, the candidate must possess a corresponding wide range of interests and expertise.

SOME REFERENCES ON THE SUBJECT

- **Charged porous media (publications of the proposers)**

K. Bourbatache, O. Millet, A. Ait-Mokhtar, Ionic transfer in charged porous media. Periodic homogenization and parametric study on 2D microstructures, *International Journal of Heat and Mass Transfer*, **55** (21-22), 5979-5991, 2012 .

K. Bourbatache, O. Millet, A. Ait-Mokhtar, O. Amiri, Modeling the Chlorides Transport in Cementitious Materials By Periodic Homogenization , *Transport in Porous Media*, **94**(1), 437-459, 2012.

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C. Moyne, M. A. Murad, Electro-chemo-mechanical couplings in swelling clays derived from a micro /macro-homogenization procedure, *International Journal of Solids and Structures*, **39**(25), 6159-6190, 2002.

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M. A. Murad, C. Moyne, A dual-porosity model for ionic solute transport in expansive clays, *Computational Geosciences*, **12**(1), 47-82, 2008.

- **Spectral methods**

J. C. Michel, H. Moulinec, P. Suquet, Effective properties of composite materials with periodic microstructure: a computational approach, *Computer Methods in Applied Mechanics and Engineering*, **172**(1-4), 109-143, 1999.

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V. Monchiet, G. Bonnet, A polarization based FFT iterative scheme for computing the effective properties of elastic composites with arbitrary contrast, *International Journal for Numerical Methods in Engineering*, **89**(11), 1419-1436, 2012.

V. Monchiet, G. Bonnet, G. Lauriat, A FFT-based method to compute the permeability induced by a Stokes slip flow through a porous medium, *Comptes Rendus Mécanique*, **337**(4), 192-197, 2009.

H. Moulinec, F. Silva, Comparison of three accelerated FFT-based schemes for computing the mechanical response of composite materials, *International Journal for Numerical Methods in Engineering*, **97**(13), 960-985, 2014.

T.-K. Nguyen, V. Monchiet, G. Bonnet, A Fourier based numerical method to compute the dynamic permeability of periodic porous media, *European Journal of Mechanics B/Fluids*, **37**, 90-98, 2013.

V.-T. To, Q.-D. To, V. Monchiet, On the inertia effects on the Darcy law: numerical implementation and confrontation of micromechanics-based approaches, *Transport in Porous Media*, **111**, 171-191, 2016.