Modeling of 2-phase flows at the pore scale in deformable media using particulate methods (SPH)

This study aims at improving the representation of gas migration in highly water saturated clays. This objective is closely related with a project to use a deep sedimentary rock formation, represented by Callovo-Oxfordian (COX) clays, as a natural barrier for radioactive waste repository. These sedimentary formations are well suited for this purpose due to low permeability of intact clayey material. However, during the post closure phase, the gas, mainly hydrogen, produced by anaerobic corrosion of iron composing many structures of radioactive wastes deep disposal may lead to important local increase of pressure, which may influence sealing properties of the repository. Various gas transport mechanisms can be active, separately or simultaneously. These include the transport of dissolved gases by advection and diffusion, the flow of small gas bubbles inside the water phase, the visco-capillary flow of gas inside the water phase, the dilatation of existing and creation of new pathways due to pressure build-up. It is well known that the major part of the porosity of clayey materials is represented by the pores of the size of a few nano-meters. Very high capillary pressure at the entry of the water saturated nano-size pores of clayey material restricts the visco-capillary and bubbly flow to largest pores. When pressure build-up grows continuously, a rapid increase of the gas flow is usually observed at a certain point, which cannot be described by standard Darcy law. It has been proposed that the gas phase migration takes place by the dilatation of existing and creation of new poral pathways. These sudden changes of the transport properties of clayey matrix necessitate coupling the two phase fluid/gas flow inside the pore space with solid matrix mechanics in order to get a better understanding of this transport mode by means of numerical simulation.

To better understand the mechanisms of gas transfer on the pore scale and to produce homogenized behavior law for use in macroscopic simulation, IRSN has recently developed simulation tool based on SPH method (Smoothed Particles Hydrodynamics), which is a Lagrangian mesh free method. Our home made SPH code allows solving, for a 3D model of porous media, the 2-phase equations of Navier-Stokes taking into account capillarity and surface tension. The solid part is being treated with the same formalism with two distinct materials: elastic part (clayly matrix) and rigid inclusions (carbonate~~s~~ or silicate~~s~~ minerals). Damage criteria (Mohr-Coulomb and Rankine) were also implemented, to control the formation of micro-fractures in the elastic part. The code was parallelized under MPI, as well as with CUDA for use on GPU.

The first part of the proposed work consists in choosing a representative model of a natural argillite based on micro-CT and SEM/FIB images which are available in our laboratory. If necessaire it will be possible to acquire additional 3d data with different spatial resolutions. Mineral phases will need to be parametrized in coherence with their respective mechanical properties.

Once the 3D model for a chosen argillite established, the next step will be to study the pertinence of the different constitutive laws with damage for the solid, elastic part. The simulation results will be compared in terms of strain, stress, gas entry pressure, and permeability with experimental results present in the literature. The student will use as a starting point the existing SPH code, which he will enrich on one hand by introducing new boundary conditions for liquids and solid, and on the other hand by implementing different damage laws.

The final part of this PhD thesis shall consist in proposing and in implementing a model of mass exchange between phases to be able to take into account the phenomena of dissolution and evaporation at the liquid-gas interface, which are very important transport mechanisms at the pore scale.

We are seeking a highly motivated student, able of independent work with a solid background in one the following domains: mechanics, physics, applied mathematics (for example in scientific computing). An experience with 2-phase flow and/or damage propagation is expected. Due to mostly numerical character of the work, the proficiency with numerical methods and programming languages (C++) would be important.

We offer a 3-years grant by IRSN, starting between October and December 2017. The thesis will take place in IRSN laboratory based in Fontenay-aux-Roses, France.

Interested candidates should contact one of the supervisors **before 1st June 2017**:

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