Modeling of thermo-hydro-mechanical couplings from pore scale to continuum with SPH method.

PSE-ENV/SPDR/LETIS

CONTENT OF THE WORK :

This project is conducted by ASNR in the frame of research in connection with the Cigéo (project for a deep geological disposal facility for HA/MAVL radioactive waste). It is particularly aimed at understanding and modelling of physico-chemical phenomena that are important for the safety of the future facility. As a significant production of hydrogen is expected inside the geological repository, this gaseous phase could modify the flows and mechanical conditions of the rock and of the engineered materials. In France, the foreseen solution is geological disposal in the Callovo-Oxfordian argillites. This argillite has a very low water permeability, porosity of the order of 20% with a connectivity controlled by pores smaller than 10 nm. Our laboratory works on different transfers and perturbations occurring in the such host-rock and develop and use a variety of direct simulation codes at several scales. We have developed a pore scale HM-gas code based on Smoothed Particle Hydrodynamics for studying water-gas migration in deformable porous media flow with drying, coupled with deformable solid (elastic with thermodynamical damage model). It is also possible to use the code for continuum simulations of hostrocks. Within EURAD 1 project (2019-2024), we developed approaches to investigate separately the impact of physical processes (mass transfer between phases: drying and condensation, hydromechanical coupling ...) involved in gas migration in hostrock at the mesoscopic scale.

In the frame of EURAD 2 (2024-2028), we will consider the coupling between the different physical (THMC) processes and upscale results at the continuum scale so that it will be possible to use them for modelling laboratory experiments from EURAD1 (some are still in progress). For upscaling process we will benefit from interaction within a dedicated work-package HERMES that will be put forward several approaches and make them interoperating. ASNR, in collaboration with GeoRessources (Univ. of Lorraine), proposes to study the THMC couplings in the near- and far-field at the micro and meso scale (order of tens of pores) based on microstructural information obtained from 3D imaging approaches (Xray µtomography, FIB-SEM, ...) within EURAD-1. Distinct but complementary numerical models (LBM: GeoRessources and SPH: ASNR) will be used for this purpose. Our work will be oriented towards taking a better profit from already implemented features in DNS (Direct Numerical Simulations) codes to improve our capabilities of simulating gas transfer in rock matrix with consideration of multiphasic features and thermal conditions including phase change and temperature dependency of multiphase flow parameters. In particular, the SPH code will be used to extensively study coupling of water-gas flow with deformation of elasto-damageable solid matrix in in-situ oriented conditions. Taking advantage from increasing capacities of modern GPUs, we will be able to simulate bigger domains and thus to compute effective properties (e.g., saturation curve, relative permeability, poromechanical properties) and their evolution with time so that an upscaled Darcy-scale model could be derived. In parallel, LBM and SPH codes are under continuous improvement to include more advanced couplings, especially energy transfer (T) and reactivity (C). Dynamics data integration though unified Hermes interface will be introduced to simulate small scale experiments in well controlled conditions.

Comparison of our computationally expensive microscale models with macroscale approaches will be used to explore the consequences of simplifying the physics and will provide benchmarking and training data for predictive surrogate models.

DESIRED SKILLS :

Modelling of two-phase flow in porous media, poromechanics, hydro-mechanical coupling, upscaling, SPH, Physics Informed Neural Networks (PINNs)

CANDIDATE BACKGROUND

PhD in numerical fluid and/or solid mechanics



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WHERE and WHEN:

Fontenay-Aux-Roses, France

Duration: 18 months (up to 21) Start: Sept-Oct 2025

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Desired skills

modelling two phase flow in porous media poromechanics C++/CUDA SPH