

Coupling classical DFT with poromechanics for adsorption-induced swelling quantification in microporous materials

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Research team	Geomechanics and Porous Media (🔗web-G2MP).
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Context

This PhD proposal is part of the I-M-API project, which aims at characterising the influence of an adsorbed phase on the instantaneous deformations in microporous media. Following the IUPAC recommendation, the pore space in porous materials is divided into three groups according to the pore size diameters: macropores of widths greater than 50 nm, mesopores of widths between 2 and 50 nm and micropores of widths less than 2 nm. Zeolites, activated carbon, tight rocks, cement paste or construction materials are among these materials. In recent years, a major attention has been paid on these microporous materials because the surface-to-volume ratio (i.e., the specific pore surface) increases with decreasing characteristic pore size. These materials can trap an important quantity of fluid molecules as an adsorbed phase. This is important for applications in gas storage, gas separation, petroleum and oil recovery, catalysis or drug delivery.

For these microporous materials, a deviation from standard poromechanics is expected. In very small pores, the molecules of fluid are confined. Fluid-fluid and fluid-solid interactions of molecules are modified and this effect may have significant consequences at the macroscale, such as instantaneous swelling deformations. In different contexts, these deformations may be critical. Generally, natural and synthesised porous media are composed of a double porosity: the microporosity where the fluid is trapped as an adsorbed phase and a meso or a macro porosity required to ensure the transport of fluids to and from the smaller pores. If adsorption in nanopores induces instantaneous deformations at a higher scale, the matrix swelling may close the transport porosity, reducing the global permeability of the porous system or annihilating the functionality of synthesised materials.

In recent years, an important effort has been involved in the modelling of the coupling between failure and transport properties in meso and macroporous media but there is still a gap to be filled between the nanoscopic scale of the pores and the macroscopic scale of the global structure in micro-to-macro materials.

Objectives & methodology

The I-M-API project aims at identifying and capturing the key couplings appearing within a nanopore and upscaling them at the scale of a structure through new enhanced poromechanical frameworks.

The final objective of the project is to obtain a robust and physically meaningful numerical simulation tool able to predict instantaneous deformation induced by an adsorbed phase in heterogeneous micro-to-macro-porous media filled with gas mixtures. Within this project, the PhD student will have to quantify and predict adsorption-induced swelling for gas mixtures in homogeneous microporous materials. For this purpose, she/he will estimate pore pressure and confinement state by the classical density functional theory and validate her/his results by using molecular simulations in collaboration with the University of Vigo, Spain. In a second step, she/he will upscale this confinement effects through the pore size distribution in an enhanced poromechanical framework for adsorption-induced swelling estimation in homogeneous materials. Finally, the model will be validated by comparisons with experimental results obtained in the lab.

Candidate's profile

The candidate should hold a master degree in physics, theoretical mechanics or a similar field. Candidates who are finalizing their master's program and will obtain their master degree in the summer of 2018 are also eligible and are strongly encouraged to apply. Previous experience with numerical simulation or modelling (thermodynamics, poromechanics, ...) is an asset. The candidate should have a strong interest in performing theoretical development and modelling. Proficiency in English is mandatory. Details available at: <http://perso.crans.org/gregoire/positions@G2MP>