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Poromechanics of microporous media

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Abstract:

Microporous media, with pores less than 2 nm large, are known to exhibit complex poromechanical behaviors because the fluid in such small pores is adsorbed and is no more bulk. Well known examples are the deformations of clay or wood induced by humidity. Much progress has been made in the recent years to understand and model the poromechanics under adsorption, and, in this presentation, I will focus more specifically on the contribution of molecular simulation. As a first approach to the problem, we will see how molecular fluctuations observed at very small scale fully characterize the poromechanics, irrespective of the nanostructure of the material. In the particular case of well-defined pore shapes (e.g., slit pores), one can define the concept of porosity, which makes it possible to develop a second approach of poromechanics, more detailed, where one distinguishes the behavior of the fluid from that of the solid. In both cases, molecular simulation is essential to capture the poromechanical effect of the fluid, at a scale hardly accessible to experiments. As illustrations, we consider the case of amorphous cellulose for the first approach and of swelling clay for the second approach.

Fluctuations of physical quantities are ubiquitous in molecular simulations at the atomic scale because of the thermal agitation. It is well known that the magnitude of the fluctuations of thermodynamic state parameters are related to the second order derivatives of the thermodynamic potential minimum at equilibrium (e.g., compressibility, thermal expansion, and heat capacity for a fluid). While fluctuation formulas are well established for simple systems (e.g., pure fluids), in the field of porous media only the isosteric heat of adsorption is commonly estimated from fluctuations, and the formula considered assumes a rigid solid. Here, we revisit the Biot-Coussy theory of thermo-poro-elasticity in a framework adapted to derive fluctuation formulas. All the thermo-poro-mechanical moduli can then be characterized by fluctuations of quantities readily accessible during a molecular simulation, i.e., with no additional computational cost and with no need to define the concepts of porosity or specific surface (ambiguous at the molecular scale). These fluctuation formulas are valid even when the fluid is adsorbed and induces unusual couplings. It is therefore possible to use the formulas to fully characterize the mechanical and thermal effects of adsorption, and conversely to characterize the adsorption response to stress and temperature. The application of these fluctuation formulas is illustrated in the case of amorphous cellulose submitted to moisture, which exhibits many unusual couplings beyond swelling (negative drained thermal expansion, very high drained heat capacity, negative Biot modulus…).

In some microporous media, such as layered clay minerals, one can define the concept of porosity and therefore distinguish between the solid and fluid phases. Doing so, it is then possible to characterize the property of the adsorbed fluid and of the solid skeleton separately. Considering the case of water confined in sodium montmorillonite, one finds that the thermo-mechanical properties are significantly affected by adsorption. Even more confusing, one finds that the Gibbs-Duhem equation no more applies, which means that the behavior of the adsorbed fluid is described by a total of 6 moduli instead of 3 for a bulk fluid. This conceptual change calls for an entirely new formulation of poromechanics. We propose such a formulation of non-linear thermo-poro-mechanics and apply it to explain two thermo-mechanical anomalies of clays: 1- the excessive thermal pressurization of interstitial water during undrained heating, and 2- the very large drained thermal expansion of over-consolidated clays. The fine analysis of these tests is quite instructive regarding the underlying physics. For instance, the excess thermal pressurization of water during undrained heating is not because bound water has a larger thermal expansion than free water (it is smaller actually), but because there is a net transfer from the bound water to the free water.

Short bio:

Laurent Brochard is a researcher at Navier lab (ENPC, Univ. Gustave Eiffel, CNRS) since 2012, and professor at École nationale des ponts et chaussées (ENPC) since 2023. He received his Ph.D. from Université Paris-Est in 2011. He is also engineer from École Polytechnique (France) and from École nationale des ponts et chaussées (France). His research focuses on multi-scale approaches for the study of the physics and mechanics of materials with emphasis on phenomena that have their origin at the molecular scale: adsorption and poromechanics, fracture mechanics and failure initiation, thermo-mechanical couplings, and confined phase transition. Targeted applications are mostly in geomechanics (CO2 sequestration, nuclear waste and energy storage, earth and bio-sourced construction, cementitious materials, and fault stability).