

Coupling between poroelasticity and the density functional theory for the estimation of adsorption-induced swelling in nanoporous materials

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Natural and synthesised porous media are generally composed of a double porosity: a microporosity where the fluid is trapped as an adsorbed phase and a meso- or a macroporosity required to ensure the transport of fluids to and from the smaller pores. In nanometer-scale pores, the molecules of fluid are confined. This effect induces that fluid-fluid and fluid-solid interactions sum at the pore scale and have significant consequences at the macroscale, such as instantaneous deformation, which are not predicted by classical poromechanics. If adsorption in nanopores induces instantaneous deformation at a higher scale, the matrix swelling may close the transport porosity, reducing the global permeability of the porous system.

This contribution aims at modelling the linear poroelastic behavior of isotropic porous media saturated with an adsorbable fluid. A poromechanical model is coupled with the molecular density functional theory (DFT) and experimental comparisons are performed in term of excess adsorption isotherms and induced strain in an activated carbon saturated with methane and carbon dioxide.

First, a version of non-local DFT [1] coupled with SAFT-VR-Mie state equation is used for the estimation of the adsorption of methane (CH₄) and carbon dioxide (CO₂) on an activated carbon. For this purpose, the material is firstly characterized by argon porosimetry at 87K to determine its pore size distribution (PSD). Thereafter, the adsorbed quantities at the pore scale are estimated for CH₄ and CO₂ respectively at 303K and 318K. The upscaling is performed through the PSD, so the adsorption isotherms are obtained and compared to experimental measurements [3].

Then, the classical poroelasticity theory is extended to consider the fluid confinement effects [2] at the nanoscale based on the DFT-SAFT estimation of the global adsorption isotherm. The estimated deformation is in good agreement with experimental measurements [3] without any fitting parameter (see Figure 1).

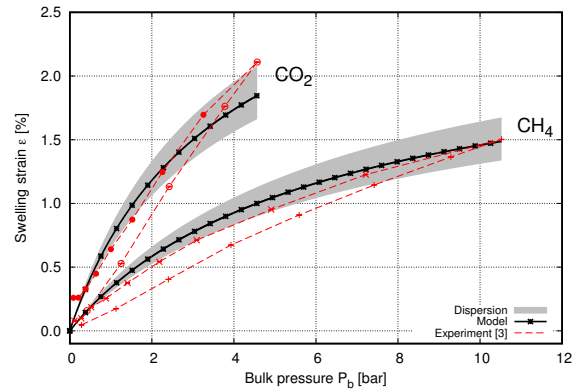


Figure 1. Comparison between swelling strain experimentally measured and estimated by the model for CH₄ and CO₂ adsorption on an active carbon.

References:

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