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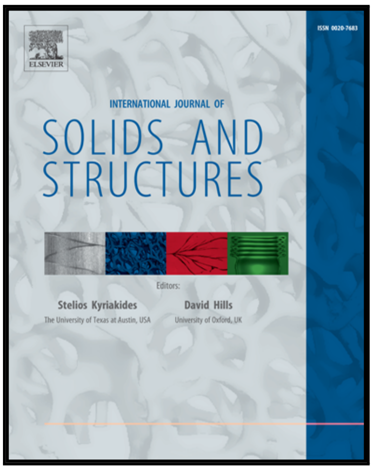

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PII: S0020-7683(18)30137-9
DOI: 10.1016/j.ijsolstr.2018.03.029
Reference: SAS 9954

To appear in: *International Journal of Solids and Structures*

Received date: 8 December 2017
Revised date: 22 March 2018
Accepted date: 29 March 2018

Please cite this article as: Laurent Perrier, Gilles Pijaudier-Cabot, David Grégoire, Extended poromechanics for adsorption-induced swelling prediction in double porosity media: modeling and experimental validation on activated carbon, *International Journal of Solids and Structures* (2018), doi: 10.1016/j.ijsolstr.2018.03.029

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Extended poromechanics for adsorption-induced swelling prediction in double porosity media: modeling and experimental validation on activated carbon

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Abstract

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 macro porosity required to ensure the transport of fluids to and from the smaller pores. Zeolites, activated carbon, tight rocks, coal rocks, source rocks, cement paste or construction materials are among these materials.

In nanometer-scale pores, the molecules of fluid are confined. This effect, denoted as molecular packing, 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 is important for applications in petroleum oil and gas recovery, gas storage, separation, catalysis or drug delivery.

This study aims at characterizing the influence of an adsorbed phase on the instantaneous deformation of micro-to-macro porous media presenting distinct and well-separated porosities. A new incremental poromechanical framework with varying porosity is proposed allowing the prediction of the swelling induced by adsorption without any fitting parameters. This model is validated by experimental comparison performed on a high micro and macro porous activated carbon. It is shown also that a single porosity model cannot predict the adsorption-induced strain evolution observed during the experiment. After validation, the double porosity model is used to discuss the evolution of the poromechanical properties under free and constraint swelling.

Keywords: Adsorption, swelling, double porosity media, poromechanical modelling

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Introduction

Following the IUPAC recommendation (Sing et al., 1985; Thommes et al., 2015), 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 (or nanopores) of widths less than 2 nm. Zeolites, activated carbon, tight rocks, coal rocks, source 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. Consequently, these materials can trap an important quantity of fluid molecules as an adsorbed phase. This is important for applications in petroleum and oil recovery, gas storage, separation, catalysis or drug delivery.

For these microporous materials, a deviation from standard poromechanics (Biot, 1941; Coussy, 2004), is expected. In nanometer-scale pores, the molecules of fluid are confined. This effect, denoted as molecular packing, induces that fluid-fluid and fluid-solid interactions sum at the pore scale and have significant consequences at the macroscale, such as instantaneous deformation. A lot of 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 deformation 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 different contexts, this deformation may be critical. For instance, *in situ* adsorption-induced coal swelling has been identified (Larsen, 2004; Pan and Connell, 2007; Sampath et al., 2017) as the principal factor leading to a rapid decrease in CO_2 injectivity during coal bed methane production enhanced by CO_2 injection. Conversely, gas desorption can lead to matrix shrinkage and microcracking, which may help oil and gas recovery in the context of unconventional petroleum engineering (Levine, 1996). The effects of adsorbent deformation on physical adsorption has also been identified by Thommes and Cychosz (2014) as one of the next major challenges concerning gas porosimetry in nano-porous non-rigid materials (e.g. metal organic framework). In conclusion,

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