



Contribution ID: 359

Type: **Poster (+) Presentation**

Two-scale poromechanical model incorporating adsorption effects of a fluid mixture in arbitrary geometrical nanopores

Thursday, 3 June 2021 20:00 (1 hour)

A two-scale poromechanical model incorporating the complex adsorption phenomena of a fluid mixture in nanopores is developed in this work. The porous medium is composed of a solid phase and nanopores of size of several nanometers where adsorption occurs. The adsorption isotherm of a fluid mixture is rigorously constructed by using the Density Functional Theory (DFT) and the Fundamental Measure Theory (FMT) [1,2] applied to a Lennard-Jones fluid. It should be noted that the studies in the literature have been limited to the case of slit, cylindrical or spherical pores [3,4,5] in which the problem can be reduced to one dimension and analytical solutions can be derived. In our work, a novel numerical method based on the Fast Fourier Transform (FFT) and 3D-voxel discretization is developed to accurately compute the fluid mixture density distributions in an arbitrary geometrical pore in three dimensions. The pore domain is firstly discretized by voxels of the same size. In this configuration, the convolution terms can be solved in Fourier space giving a huge advantage in terms of time calculation and computer resources. Numerical simulations show the density profiles of CH₄ and CO₂ gas mixture in an ellipsoidal pore, considering the fluid-fluid and solid-fluid Lennard-Jones interaction-types, highlighting the potential of the current method. Such approach is capable of computing accurately the adsorbed gas densities in any pore geometry, regardless of the difference of molecule diameters.

Given the gas densities, the solvation force, which is the force exerting on the solid wall by the fluid phase in arbitrary geometrical nanopores, is then computed by using a new derived formulation obtained from mechanics and thermodynamics approaches. It is important to notice that the solvation force in the pore is normally negative and its order of magnitude is much higher than the bulk pressure, leading to an important impact on the mechanical properties at higher scale. To consider this force in the poromechanical model, the local mechanical description at the pore scale is upscaled to the macroscale by using the homogenization technique in the sense of [4,5]. As a result, the macroscopic total stress tensor is the sum of a classical elastic part and a solvation component due to the solvation force which acts as a pre-stress inside the material. This analysis allows accurately predicting the volumetric strain of the medium with respect to variation in pressure and gas composition. Numerical simulations show an application to coalbed methane, predicting the coal matrix swelling with the increase in gas pressure. It is highlighted that the adsorption potential of CO₂ is higher than the one of CH₄, therefore the volumetric strain due to the increase in CO₂ pressure is much more significant.

Time Block Preference

Time Block B (14:00-17:00 CET)

References

[1] Y. Rosenfeld, Free-energy model for the inhomogeneous hard-sphere fluid mixture and density-functional theory of freezing, *Physical Review Letters*, 63, 980-983 (1989).

[2] E. Kierlik and M. L. Rosinberg, Density-Functional theory for inhomogeneous fluids: adsorption of binary-mixtures, *Physical Review A*, 44, 5025–5037 (1991).

[3] A. Gonzalez, J. A. White, F. L. Roman, and S. Velasco, Density functional theory of fluids in nanopores: analysis of the fundamental measures theory in extreme dimensional-crossover situations, *The Journal of Chemical Physics*, 125, 64703- (2006).

[4] T. D. Le, C. Moyne, M. A. Murad, I. Panfilov, A three-scale poromechanical model for swelling porous media incorporating solvation forces: Application to enhanced coalbed methane recovery, *Mechanics of Materials*, 131, 47-60 (2019)

[5] T. D. Le, H. Q. Dat, I. Panfilov, C. Moyne, Multiscale model for flow and transport in CO₂-enhanced coalbed methane recovery incorporating gas mixture adsorption effects, *Advances in Water Resources*, 144, 103706- (2020)

Acceptance of Terms and Conditions

[Click here to agree](#)

Newsletter

Student Poster Award

Primary authors: Mr HA, Quoc Dat (LEMTA, Université de Lorraine, CNRS); Prof. LE, Tien Dung (LEMTA, Université de Lorraine, CNRS); Prof. PANFILOV, Irina (LEMTA, Université de Lorraine, CNRS); Prof. MOYNE, Christian (LEMTA, Université de Lorraine, CNRS)

Presenter: Mr HA, Quoc Dat (LEMTA, Université de Lorraine, CNRS)

Session Classification: Poster +

Track Classification: (MS13) Fluids in Nanoporous Media