Simple Fluids confined in Nanopores: from local transport properties to shear-swelling couplings

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1 Introduction

Dense fluids confined between flat solid surfaces are generally strongly inhomogeneous in the direction normal to the fluid-solid interfaces due to surface effects (layering of the molecules of the fluid because of adsorption and molecular packing) [1]. Thus, when the solid surfaces are separated by a distance that is smaller than about 10 times the molecular diameters of the fluid, the confined fluid exhibits local and effective transport properties that may strongly differs from those of the bulk [1-3]. Furthermore, this extreme confinement can induce as well strong forces (solvation) on the solid matrix that may lead to swelling/shrinkage as well known in clays for instance.

2 Methods and models

To improve the microscopic understanding of the phenomena described above, we have performed extensive molecular dynamics simulations on simple fluids confined between flat solid surfaces. In all cases the solid phase has been modeled using a rigid CFC crystal composed of Lennad-Jones atoms.

Concerning the fluid, different molecular models were employed, from hard sphere to Lennard-Jones, so as to build new weight functions for a non-local model for transport properties based on a local average density model. Furthermore, to ensure the reliability of the model so obtained, various thermodynamic conditions have been explored.

Various non equilibrium molecular dynamics scheme have been developed [2-4], see Fig. 1, in order to study the impact of extreme confinement of the dynamic fluid properties.

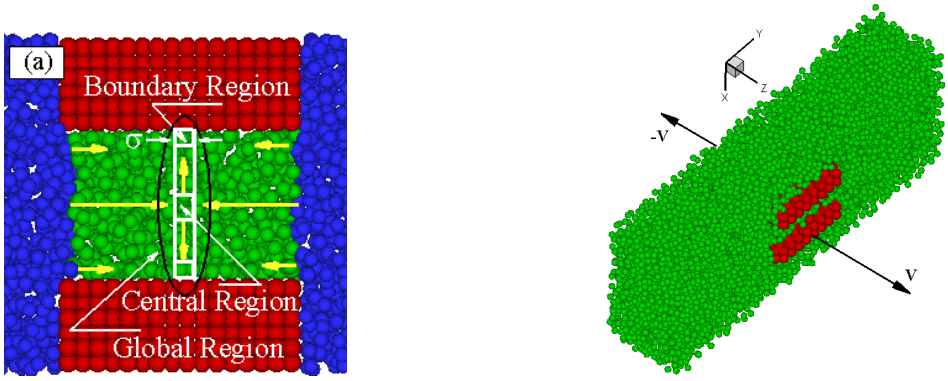

Figure 1: *Left:* Scheme of the molecular dynamics simulation used to study unsteady mass diffusion (blue and green: fluid particles of two species, red: solid particles) in a nanopore. *Right:* Scheme of the molecular dynamics simulation cell used to study couplings between shear and swelling (green: fluid particles, red: solid particles).

3 Discussion

In the first part of the presentation, we will show how the local variations of the transport properties of the confined fluid (diffusion [1], viscosity [2]), induced by density inhomogeneities, can noticeably affect the effective transport properties of the fluid quantified at the pore scale. Furthermore, it will be shown that these local transport properties can be essentially described by a simple local average density model combined with simple weight functions [3], see Fig. 2.

In the second part of the presentation, we will discuss the couplings that occur between shear and swelling at the pore scale because of the strong fluid structure [4]. It will be shown that shear can induce swelling and vice versa because of the confined fluid phase structure, see Fig. 2. This implies that the response to a variation of the external load is a combination of volumetric and shear deformations, because of the fluid.

These phenomena, which are usually neglected in poromechanics modeling, may be non-negligible in highly structured microporous systems such as cementitious or clay-based materials [5].

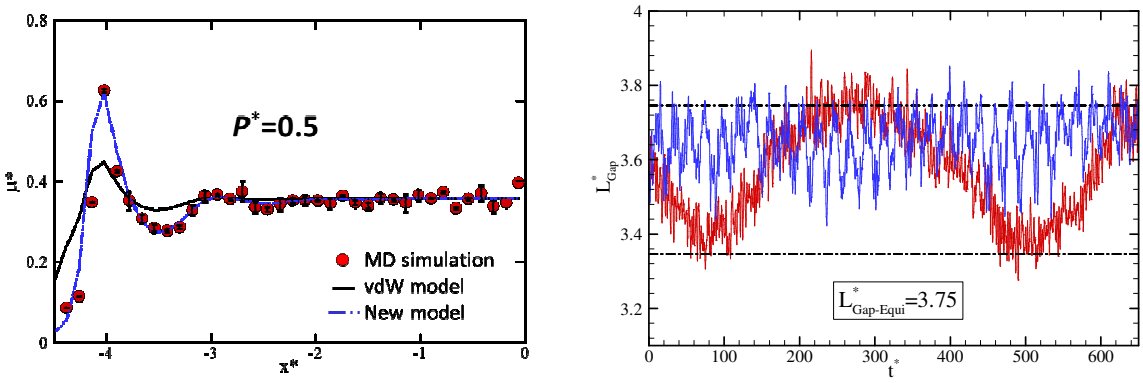

Figure 2: *Right*: Variation of the local shear viscosities perpendicularly to the solid wall. *Right*: Variation of the distance between the solid surfaces with time during boundary shear.

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