Perméation de gaz à travers une constriction nanoporeuse : théorie et simulations

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Permeation of gas through nanoporous constrictions : theory and simulations

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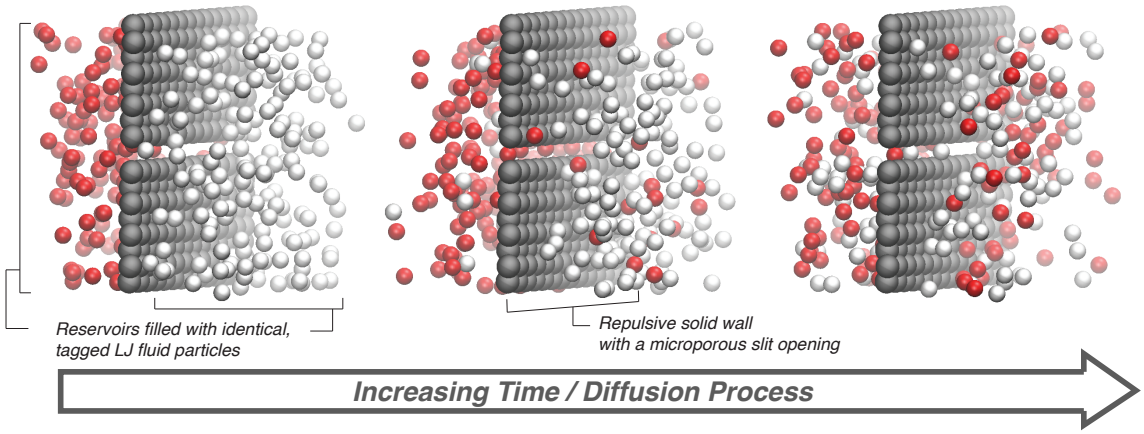

Figure 1: Principle of our Molecular Dynamics numerical experiment

Fluid transport through carbon-based materials has several applications among which design of nanoporous carbons for gas separation, production of gas from shales and coal seams or geological CO2 sequestration. The determination of transport properties in such media is therefore of great interest. In the context of carbon membranes, numerous experimental studies have reported the dependence of permeation and separation properties on thermodynamic conditions (pressure, temperature) and properties of the system (fluid species, structural properties of the membrane, etc) [1]. Recently, Botan et al. performed molecular simulations that reproduced some typical features of the experimental results found in the literature [2]. More precisely, these authors evidenced that steric effects inherent to fluid permeation through molecular size constrictions drive the overall transport properties of the membrane. The present work focuses on molecular simulations of fluids permeating through single nanoporous constrictions. As a first approach, our molecular model consists in a monoatomic thick wall connecting two independent fluid reservoirs via a nanoporous slit (see 1). We report how permeation rates depend on several parameters, such as the size of the slit, thermodynamic conditions and the amplitude of molecular interactions. By means of simple theoretical models that reproduce our simulations data, we shed light on the range of mechanisms that rule molecular permeation through nanoporous constrictions. We believe our results are of practical interest for the design of architectured nanoporous materials such as nanoporous graphenes.

References

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