CONFLUENCES IMFT

Institut de Mécanique des Fluides

Amphithéâtre Nougaro (Entrée A) - 2 Allée du Pr Camille Soula, Toulouse

Mercredi 21 Mars - 10 h 30

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Molecular Dynamics simulations: A complementary tool to better model fluids behavior

Classical Molecular Dynamics simply consist in simulating the evolution over time of a set of model molecules interacting with each other's. From these simulations, it is then possible to compute all emerging physical properties and fields of the simulated materials. These numerical tools have proved usefulness both in assisting theoretical developments on thermophysical properties modelling and in providing pseudo-experimental data in situations where experiments are difficult to perform [1].

In this presentation, we will focus on some fundamental and applied examples on what has been done in our group with these numerical tools to better understand and quantify heat, mass and momentum transfers at interfaces and in low permeability media [2-4]. These examples will concern slip at fluid-solid and fluid-fluid interfaces, modification of effective transport properties under confinement, multicomponent transport, thermogravitation ... and will illustrate the possibilities, and limitations, of the use of molecular simulations to enhance classical macroscopic modelling.

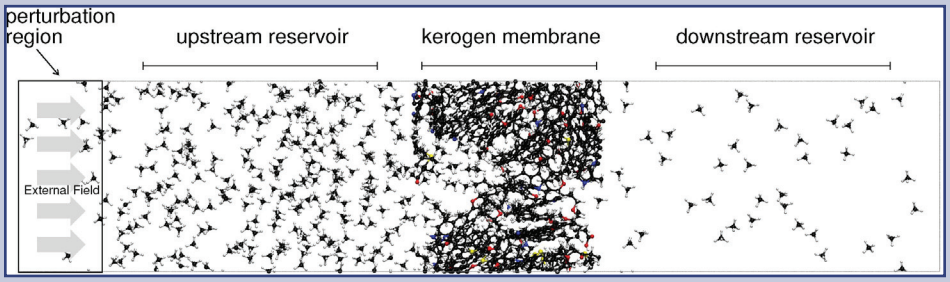

Figure: Transport of gas through a type II kerogen membrane

REFERENCES

[1] G. Galliero, in M. J. Assael, A. R. H. Goodwin, V. Velisovic, W. A. Wakeham, eds, Experimental Thermodynamics Volume IX: Advances in Transport Properties of Fluids, Royal Society of Chemistry, London, 2014, Chapt. 11, pp. 362-386.
[2] H. Hoang, G. Galliero, Phys. Rev. E 86, 021202 (2012)
[3] J. Collell et al., J. Phys. Chem. C 119, 22587 (2015)
[4] G. Galliero et al., NPJ Microgravity, 3, 1 (2017)

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