Adsorption and Transport in Hierarchical Nanoporous Media

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Hierarchical nanoporous materials, which combine several porosity scales, are widely used in industry (adsorption, separation, catalysis) to overcome slow diffusion and enhance access to the large surface area in microporous solids (< 2 nm). The benefits of adding meso (2-50 nm) and macro (> 50 nm) pores to the existing microporosity was demonstrated but engineering of such solids, which are heterogeneous in size, shape, and connectivity, still relies on trial and error strategies. Available modeling approaches, even when based on a physical ground, are limited to empirical parameters which cannot be derived from molecular adsorption/transport coefficients. In particular, none of the existing approaches offers the ground for a bottom up model of adsorption/transport in multiscale materials as (1) they describe empirically the interplay adsorption/transport and (2) they do not account for the breakdown of hydrodynamics at the nm scale.

I will present a multiscale model of adsorption and transport in hierarchical nanoporous materials (Figure 1) [1]. I will first show how adsorption, permeance, and transport in such media can be described without having to rely on macroscopic concepts such as hydrodynamics [2,3]. Using fundamental parameters and coefficients available to simple experiments, we will see how transport coefficients can be rigorously obtained from simple models in the framework of Statistical Mechanics. Then, I will present a multiscale model of adsorption and transport in hierarchical materials [4]. Thanks to the use of atom-scale simulations, which capture the different adsorption and transport regimes upon varying the temperature, pore size, pressure, etc. this bottom-up model does not rely on hydrodynamics and, hence, does not require assuming a given adsorption or flow type. I will also discuss NMR experimental results on transport in hierarchical zeolites [5].

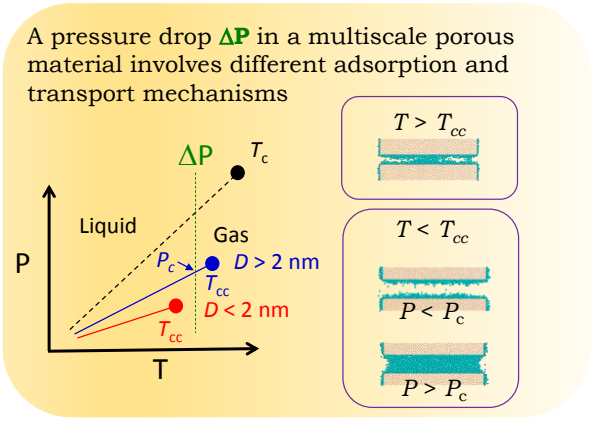

Figure 1 : P-T phase diagram of a fluid confined in micro and mesopores. For a pore size D, the bulk critical temperature T_c is shifted to $T_{cc}(D)$. Pore filling is reversible for $T > T_{cc}$, and irreversible for $T < T_{cc}$. In the latter case, the pore is partially filled for $P < P_c$ and completely filled for $P > P_c$.

[1] B. Coasne, A. Galarneau, C. Gerardin, F. Fajula, F. Villemot, Langmuir 29, 7864 (2013).
[2] K. Falk, B. Coasne, F. J. Ulm, R. Pellenq, L. Bocquet, Nature Comm. 6, 6949 (2015).
[3] T. Lee, L. Bocquet, B. Coasne, Nature Comm. 7, 11890 (2016).
[4] A. Botan, F. J. Ulm, R. Pellenq, B. Coasne, Phys. Rev. E 91, 032133 (2015).
[5] A. Galarneau, F. Guenneau, A. Gedeon, D. Mereib, J. Rodriguez, F. Fajula, B. Coasne, J. Phys. Chem. C 120, 1562 (2016).