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**Retarded desorption from porous media caused by wetting/dewetting of the external surface** THOMAS LEE, BENOIT COASNE, ROLAND J.-M. PELLENQ, FRANZ-JOSEF ULM, Department of Civil and Environmental Engineering, Massachusettes Institute of Technology, Cambridge, MA, LYDÉRIC BOCQUET, Laboratoire de Physique Statistique, Ecole Normale Supérieure, Paris, France, MULTISCALE MATERIAL SCIENCE FOR ENERGY AND ENVIRONMENT COLLABORATION[1] — Despite the increasing attention devoted to nanofluidics, the role of external surfaces on transport in nanopores has not been fully investigated. Here, we report molecular dynamics simulations showing that methane recovery from a hydrophobic nanoporous membrane is retarded by the presence of liquid water at the external surface. Despite the pressure gradient used to trigger methane desorption and the hydrophobicity of the membrane, methane remains trapped for long times until water desorbs from the external surface. Using umbrella sampling calculations, we show that this retardation effect is induced by the free energy cost of dewetting the external surface as water is replaced by an adsorbed methane film. To account for this effect, we propose a simple thermodynamic model which describes the increase in free energy during extraction (dominated by the large methane-water surface tension). We also extend our approach to hybrid external surfaces made up of hydrophilic/hydrophobic regions, and consider fluids other than water ($CO_2$), as these are relevant to practical applications such as gas/oil recovery from shale. Such retarded processes also have implications for transport in nanofluidic systems and adsorption/transport in solid catalysts, chromatographic devices, etc..

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