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Molecular Simulation and Theory of Gas Transport across Thin Liquid Films
Long Master Thesis / Master Nanosciences - Nanotechnology

Gas separation refers to filtering techniques that are used to give multiple gaseous products or to purify a single gaseous product. Among various techniques, pressure swing adsorption pressurizes and depressurizes gases in a solid porous membrane to selectively adsorb some components. These membranes act as permeable barriers through which compounds are separated because they move at different rates depending on- their size, diffusivity, and solubility into the membranes. Despite advantages such as their high selectivity and regeneration ease, liquid membranes have received far less attention than solid membranes[1]. In particular, while supported soap films have been studied[2,3], **self-standing soap films** have never been considered for gas separation despite (1) a large active surface area increasing the separation throughput, (2) a chemical composition maintained constant due to flow, and (3) the possibility to destroy and reform them easily thus circumventing the problems associated to the poisoning of the surfaces.

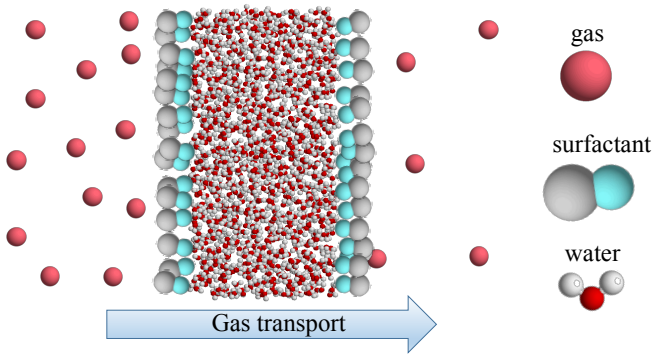

Fig. 1. Gas transport across a thin water film stabilized by surfactant molecules (soap film). (*left*). While water is described using a molecular model, the gas and surfactant molecules can be described using coarse-grained models (*right*).

In this long master thesis, we propose to investigate by means of molecular simulation liquid films as gas separation devices (**Fig. 1**). First, Monte Carlo simulations combined with free energy calculations will be used to determine the thermodynamics of various gases (typically CO_2 and Methane) crossing a water thin film stabilized by surfactants. These simulations will provide thermodynamic properties such as gas selectivities (concentration ratio inside and outside the film) at different pressures and free energy barriers limiting gas transport across gas/liquid interfaces[4]. Then, using Molecular Dynamics simulations, transport properties such as the self/collective diffusivities and permeability of the liquid foam films for each gas compound will be determined[5]. *Although dedicated to theoretical aspects, this master thesis will be performed in the frame of an experimental/theoretical project supported by the TEC21 Laboratory of Excellence in Grenoble. No specific computer skills are required to perform this master thesis but the student will have to learn and write their own analysis codes (Monte Carlo and Molecular Dynamics codes will be provided).*

[1] F. F. Krull, C. Fritzmann, T. Melin, *J.Membr. Sci.* **325**, 509 (2008).
[2] K. Setnickova, V. Sima, R. Petrychkovych, J. Reznickova, P. Uchytil, *Sep. Pur. Tech.* **160**,132 (2016).
[3] M. Ramanathan, H.–J. Muller, H. Möhwald, R. Krastev, *Appl. Mat. Int.* **3**,633 (2011).
[4] T. Lee, L. Bocquet, B. Coasne, *Nature Comm* **7**, 11890 (2016).
[5] K. Falk et al. B. Coasne, R. Pellenq, F. –J. Ulm, L. Bocquet, *Nature Comm.* **6**, 6949 (2015).