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Surfactant Adsorption in Porous Media

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Internship at the Master 2 level at LIPhy/Grenoble

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Surfactants are important in soft matter physics. These amphiphile molecules, which possess a hydrophilic head combined with a hydrophobic tail, are relevant to many applications such as soap films, detergents, cosmetics, depollution, etc. Besides their ability to decrease surface tension by getting adsorbed at interfaces, an important property of surfactants in water is to exhibit a complex phase diagram including a miscibility gap – there is a range of temperature/concentration where demixion occurs from water. Even in the miscibility region, there exists a *critical micelle concentration* (CMC) above which surfactants form a micelle – typically spherical micelles where the surfactant tails tend to lie parallel inside the micelle while polar or charged heads are at the micelle external surface in contact with water (**Fig. 1**).

The tendancy to form micelles can be used for many applications, especially in heterogeneous solutions such as oil/water systems to trap oil droplets inside the core of surfactant micelles. In many/most situations, such phase separation occurs or is performed in **porous media**; an important example being the use of surfactants to untrap important oil amounts located in oil reservoirs/rocks. In this Master 2 internship, we propose to use statistical mechanics to investigate from a theoretical standpoint the role of **confinement and surface forces** – that are inherent to porous media – on the phase diagram of surfactants. More in detail, an extended Ising lattice model[1] will be used to investigate the effect of pore size and surface molecular interactions on **surfactant adsorption and micellization in porous media** (**Fig. 2**). We will first consider simple pore geometries (slit, cylinder) to assess first order effects before moving to disordered porous media to consider more realistic situations. This internship is dedicated to fundamental physics but will be performed in strong connexion with IFP Energies Nouvelles, therefore offering an ideal opportunity to apply robust statistical mechanics to a complex multiscale problem relevant to industrial applications.

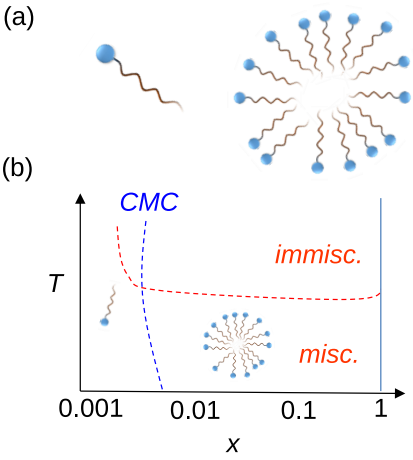

Fig. 1. (a) Surfactant molecule exhibiting a hydrophilic head (blue sphere) and a hydrophobic tail (grey chain). (b) Schematic temperature/concentration phase diagram of surfactants in water. Surfactants in water are either miscible or immiscible with a miscibility gap shown as the red dashed line. Even in the miscibility range, there is a critical concentation (CMC) above which surfactants form micelles.

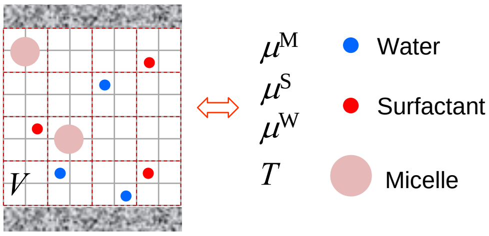

Fig. 2. Statistical mechanics model of surfactant adsorption and phase diagram in porous media. The different species (water, surfactant, and micelle) are confined between two surfaces (grey rectangles) forming a slit pore. The system has a constant volume and is in equilibrium with an infinite reservoir imposing its temperature and chemical potentials.

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[1] H. Bock, K. E. Gubbins, *Phys. Rev. Lett.* **92**, 135701 (2004).