

Ph.D. defense

Institut de Chimie Séparative de Marcoule / CEA Marcoule
(UMR 5257, CEA, CNRS, Université Montpellier, ENSCM)

LOLITA HILAIRE

will present her Ph.D. dissertation

Coalescence modelling: connecting scales (from a deterministic approach to a stochastic one)

The defense will take place on **Thursday, February 17, 2022 at 9.30 am**
in the ICSM Auditorium

In order to respect the procedures for organizing public events in the ICSM auditorium, people who wish to attend the thesis can register before by sending an e-mail to jean-francois.dufreche@icsm.fr. The health pass and the surgical mask are mandatory.

Coalescence plays a fundamental role in many industrial processes such as liquid-liquid extraction. It is a complex multi-scale phenomenon that relies on the interaction between deformable droplets that might be subjected to a flow. However, the coalescence process remains poorly understood, especially at the nanoscale. In this thesis, coalescence is studied at the molecular scale by means of molecular dynamics simulations in order to connect the different scales.

The first axis deals with the interaction between an AFM tip and a liquid film deposited on a substrate. This is a simple case compared to the liquid-liquid coalescence because one of the droplets (the AFM tip) is rigid, and the intermediate medium is gaseous. The results show that the surface fluctuations cause an instability of the interface deformation and are responsible of the jump-to-contact phenomenon in which the liquid comes into contact with the tip. Our results, on an experimentally observable system, have confirmed the validity and the limitations of continuous models. The second axis concerns the study of the drainage of the interfacial film. An original approach is proposed, in which planar layers of water and heptane are constructed and stacked under periodic conditions. The two liquids are subjected to flows in opposite directions. The velocity profiles obtained in the molecular dynamics simulations are used to assess the effective viscosity of films confined between two liquid phases and to study the slip at the interfaces. Our results show that there is a significant slip at the liquid-liquid interface. The ratio of the slip lengths is equal to the ratio of the respective viscosities of the two liquids. This slip located at the liquid-liquid interfaces plays an important role during coalescence since it accelerates the film drainage. Finally, we study the stochastic effects controlling the formation of the liquid bridge through a series of simulations of coalescence of heptane drops in water. The simulation box is the same in each case, but a random perturbation is introduced by the Lyapunov instability, allowing the obtention of a set of closely related initial states having divergent trajectories. From this series of simulations, we have established that the probability of coalescence as a function of time follows a Poisson distribution.

In summary, we have proposed an original description of coalescence at the molecular scale using a probabilistic model describing the coalescence time and a hydrodynamic model describing the drainage at the molecular scale. Our study opens many perspectives for the simulation of coalescence in continuous approaches used in fluid mechanics and chemical engineering. It is also applicable to other physical problems whose kinetics are governed by the molecular scale.

Keywords: Droplet coalescence; Molecular Dynamics; Physical chemistry of interfaces; Liquid-liquid flow; Modelling

