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Binary mixtures thin films stability : some insights from molecular simulations

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Thin liquid films play a key role in many natural phenomena and technological applications. So far, a lot of studies have been made on this topic from a macroscopic hydrodynamic perspective. However, for example, in the case of foam films, it is reported that the theoretical values of the critical thickness of the foam films are lower than the ones measured experimentally [1,2]. In this regard molecular dynamics simulation is a very interesting numerical tool both testing existing models and to have access to information that are not available from an experimental point of view.

Within that framework, the stability of thin liquid films was studied in the case of binary mixtures composed of alkane and aromatic. In such systems, two competing mechanisms are expected to occur. The first one is the attraction between the two interfaces that will lead to a thinning of the film. However, in the case of mixtures, this tendency to thinning may be compensated by a reorganization of species at the interfaces which will result in an increase of the surface tension and therefore may enhance the lifetime of the liquid film. Such enhanced liquid film lifetimes have already been observed in some experimental works and have been convincingly explained by the previously described mechanism [3]. To shed further light on such a mechanism at the microscopic scale and to better quantify it, molecular simulations have been performed on thin liquid films of various widths composed of normal alkane and aromatic mixtures. By doing so, as it will be shown, it is possible to have access to information (like the distribution of the species in the interfaces, or the local contribution to the tension along the simulation box) that may help in better understanding the underlying physical mechanisms at play.

[1] Manev, E.D.; Angarska, J.K. Critical thickness of thin liquid films: Comparison of theory and experiment.Colloids Surf. A Physicochem. Eng. Asp.2005,263, 250–257
[2] Ivanova, D.S.;Angarska, J.K. Drainage and critical thickness of foam films stabilized byn-dodecyl-β-D-maltoside.Colloids Surf. A Physicochem. Eng. Asp.2013,438, 93–103
[3] H.-P. Tran, M. Arangalage, L. Jørgensen, N. Passade-Boupat, F. Lequeux, and L. Talini Understanding Frothing of Liquid Mixtures: A Surfactantlike Effect at the Origin of Enhanced Liquid Film Lifetimes P
hys. Rev. Lett. 125, 178002 (2020)