Theoretical approaches to cavitation in confined conditions

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Today, the common trend to deal with cavitation in confined systems is to rely on detailed numerical simulations. Due to their high computational cost, these simulations are however limited to simple geometries, such as a single pore ink-bottle shaped, and cannot be extended to more complex geometries, such as disordered porous glasses. One of the goals of the ANR CAVCONF is to go beyond this limitation.

In this contribution, we first present a simplified model of cavitation in confined geometries. This new model extends the Saam and Cole's model [1] of adsorption and desorption in a single cylindrical pore to the case of finite thermal activation. It thus describes activated nucleation for condensation, and cavitation for evaporation, generalizing in the latter case the Classical Nucleation Theory (CNT) by including the effect of the fluid interaction with the walls. In the CAVCONF project, we aim to compare the predictions issued from this model to experimental results for helium and nitrogen, so as to assert its validity for simple fluids in large enough cavities. This approach has however limitations, in particular with respect to the continuum (macroscopic) description of the fluid. This led us to develop at ICMN numerical simulations based on a realistic atomistic modelisation of the fluid, allowing to tackle issues like the influence on cavitation of the fluid structure near the solid, or the influence of the solid heterogeneity on cavitation. This approach is also well suited to study more complex fluids, in particular polar molecules such as water, or linear molecules such as alkanes. We will describe the first results of this approach.

[1] W. F. Saam and M. W. Cole. Excitations and thermodynamics for liquid-helium films. Phys. Rev. B, 11, 1086–1105, (1975).