Evaporation of free and sessile droplets at mesoscale

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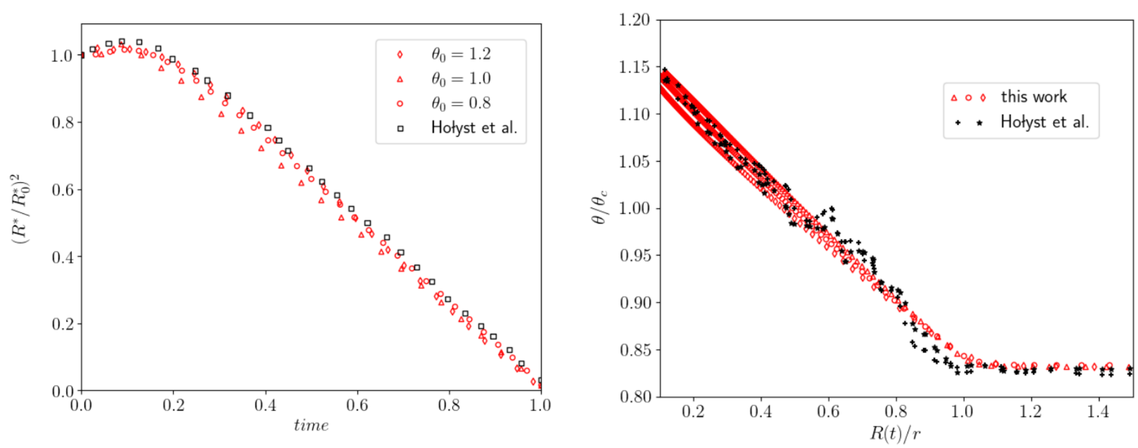
Evaporation plays a crucial role in both natural phenomena and technological applications, including cooling systems, coating processes, and biomedical technologies. Despite significant advances, the complexity of droplet evaporation still poses fundamental challenges. For instance, its inherently multi-scale nature limits a comprehensive understanding both experimentally and numerically. In particular, the presence of a solid substrate introduces additional complexities due to fluid-solid molecular interactions, which influence the overall hydrodynamics of the evaporation process.

To address these challenges, we employ a diffuse interface model to investigate the evaporation of both freely suspended spherical droplets and sessile droplets at submicron scales[1]. The spherical droplet case is analyzed across different size ranges, from molecular scales, where results are directly compared with molecular dynamics (MD) simulations[2], to larger droplets approaching the macroscopic regime. The model exhibits excellent agreement with MD results, Figure 1, and accurately captures evaporation dynamics across scales, intrinsically accounting for variations in thermodynamic properties.

For sessile droplets, evaporation occurs in constant contact angle mode, with substrate wettability and temperature significantly affecting the process. Lower wettability and higher temperatures enhance the evaporation rate, while substrate superheating causes the apparent contact angle to deviate from the equilibrium value imposed by the substrate. At sufficiently high superheating, the Leidenfrost effect occurs, leading to the formation of a vapor film at the liquid-solid interface and a reduction of the evaporation flux.



(a) (b)

Figure 1: Comparison between the simulation results (red symbols) and those from MD simulations (black symbols): a) Evolution of the square-equivalent radius, $R(t)^* = R(t)^2(1 - 2/3.R(t)/R_\mathrm{b})$, normalised by its initial value. b) Temperature distribution results within the domain.

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[1] M Gallo et al., *Journal of Fluid Mechanics* **906** (2021).

[2] R. Holyst and M. Litniewski., *Physical review letters* **100(5)** (2008).