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Challenges of modelling the moving contact line problem and recent progress: bridging scales from the nano- to the macroscale

The moving contact line problem occurs when modelling one fluid replacing another as it moves along a solid surface, a situation widespread throughout industry and nature. Classically, the no-slip boundary condition at the solid substrate, a zero-thickness interface between the fluids, and motion at the three-phase contact line are incompatible - leading to the well-known shear-stress singularity. At the heart of the problem is its multiscale nature: a nanoscale region close to the solid boundary where the continuum hypothesis breaks down, must be resolved before phenomenological macroscale parameters such as contact line friction and slip, often adopted to alleviate the singularity [1], can be obtained.

Here we will review progress made by our group considering the moving contact line problem and related physics from the nano- to macroscopic lengthscales. Specifically, to capture nanoscale properties very close to the contact line and to establish a link to the macroscale behaviour, we employ elements from the statistical mechanics of classical fluids, namely density-functional theory (DFT) [2,3]. We formulate a new and general dynamic DFT (DDFT) [4]that carefully and systematically accounts for the fundamental elements of any classical fluid and soft matter system, a crucial step towards the accurate and predictive modelling of physically relevant systems. In a certain limit, our DDFT reduces to a non-local Navier-Stokes-like equation [5]: an inherently multiscale model, bridging the micro- to the macroscale, and retaining the relevant fundamental microscopic information (fluid temperature, fluid-fluid and wall-fluid interactions) at the macroscopic level.

Work analysing the contact line in both equilibrium and dynamics will be presented [6,7]. The new model allows us to benchmark existing phenomenological models and reproduce some of their key ingredients. But its multiscale nature also allows us to unravel the underlying physics of moving contact lines, not possible with any of the previous approaches, and indeed show that the physics is much more intricate than the previous models suggest. For instance, a key property captured by our theory is the fluid layering on the wall-fluid interface, amplified as the contact angle decreases. But also the existence of compressive interfacial regions on the vapor side of the vapor-liquid interface and a large-shear region close to the wall in which effective slip can be generated. We demonstrate that the stratified fluid structure in the vicinity of the wall has a large effect on the compression and shearing properties of the fluid. We also scrutinize the effect of stratification on contact line friction and the dependence of the latter on the imposed temperature of the fluid and motion orientation [8].

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