A Study of Fluid Interfaces and Moving Contact Lines Using the Lattice Boltzmann Method

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Abstract. We study the static and dynamical behavior of the contact line between two fluids and a solid plate by means of the Lattice Boltzmann method (LBM). The different fluid phases and their contact with the plate are simulated by means of standard Shan-Chen models. We investigate different regimes and compare the multicomponent vs. the multiphase LBM models near the contact line. A static interface profile is attained with the multiphase model just by balancing the hydrostatic pressure (due to gravity) with a pressure jump at the bottom. In order to study the same problem with the multicomponent case we propose and validate an idea of a body force acting only on one of the two fluid components. In order to reproduce results matching an infinite bath, boundary conditions at the bath side play a key role. We quantitatively compare open and wall boundary conditions and study their influence on the shape of the meniscus against static and lubrication theory solution.

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1 Introduction

The motion of the contact line, the common borderline between a solid, a liquid, and its equilibrium vapor, is key to several important applications like coating, painting or

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oil recovery [1-3]. The dynamics of the contact line has stimulated theoretical studies and experimental investigations [4-9]. The dynamics is controlled by a rather subtle competition between the interfacial interactions amongst three phases, the dissipation in the fluid, and the geometrical or chemical patterning and irregularities of the surface. The first fundamental steps in the field are due to Landau and Levich [10] and to Derjaguin [11], who studied the problem of liquid film coating on a perfectly wetting substrate; this problem is referred to as the "LLD problem" hereafter. In the case of perfect wetting, one observes a film deposition whose thickness is controlled by the balance between viscous forces and surface tension. The solution of the LLD problem is an example of matched asymptotic between the static capillary meniscus and the liquid film (LLD film). It is well known that in a continuum description the viscous forces would diverge at the contact line [12], a problem commonly referred to as the "viscous singularity". In nature the viscous singularity is resolved by the presence of some microscopic cutoff scale, l_s , (e.g. the size of a liquid molecule) while in numerical approaches a cutoff is also invariably introduced, e.g. the size of the discretization mesh. Far from the contact line, viscous forces are negligible and the shape of the static capillary meniscus is set by the balance between gravity and surface tension.

The problem of liquid film entrainment was further investigated by de Gennes [13] for the case of partial wetting. When the liquid partially wets the plate with a non-vanishing dynamic contact angle, a steady state is achieved only for plate velocities smaller than a certain critical value. More recently it was shown that partial wetting substrates allow for the existence of a second admissible solution for the thickness of the film [8] and it was shown experimentally that in the case of non-wetting fluids a remarkable ridge-like structure is produced during the entrainment process [9]. The solution of the LLD problem has also been generalized to non-Newtonian "power law" fluids by Tallmadge [14], plastic-viscous fluids by Deryaguin and Levi [15], to include the effects of inertia by de Ryck and Quere [16], as well as the effects of Marangoni stresses by Ramdane and Quere [17].

Another case of interest is when the solid plate is plunged into the bath instead of being pulled; in the present manuscript this problem is referred to as plunging plate problem. When pulling the plate a liquid film entrainment is easily attained even at small velocities however, for case of a plunging plate this requires considerably higher velocities [18].

In the present manuscript we show numerical simulations based on the multiphase and multicomponent versions of the Lattice Boltzmann method to investigate its applicability to study the dynamics of the three phase contact line. Further, we quantitative investigate and discuss the role of boundary conditions. In Fig. 1 we report the schematic of the setup that we consider. The fluids with dynamic viscosities $\mu_1 = \rho_1 \nu_1$ and $\mu_2 = \rho_2 \nu_2$ ($\mu_2 \le \mu_1$ and we define $R = \mu_2/\mu_1$) are separated by an interface. At the top and at the bottom boundaries we mimic an infinite bath by imposing "flux" boundary conditions (described in Section 4). The flux boundary conditions are used to sustain the hydrostatic pressure of the liquid column in the domain. At the left boundary we impose a no-slip