Numerical simulations of 3D flows with moving contact lines

Z. SOLOMENKO[a], P. D.M. SPELT[a], J. F. SCOTT[a]

a. Laboratoire de Mécanique des Fluides et d'Acoustique, École centrale de Lyon – CNRS – Université Claude Bernard Lyon 1 – INSA Lyon, 36 avenue Guy de Collongue, 69134 Écully cedex, France
zlatko.solomenko@ec-lyon.fr

Résumé

Un solveur diphasique a été développé pour simuler les grandes échelles d'écoulements avec lignes de contact dynamiques. La dynamique de la ligne de contact est prise en compte en utilisant un modèle sous-maille basé sur des théories hydrodynamiques. Le code a été validé à partir de données expérimentales et numériques pour des écoulements axisymétriques et 3D sur des supports plans homogènes.

Abstract

A two-phase flow solver has been developed to simulate 3D large-scale flows with moving contact lines. Contact line dynamics is taken into account using a subgrid model based on hydrodynamic theories. The code has been validated against existing experimental and numerical results, for axisymmetric and 3D flows on planar homogeneous substrates.

Keywords: hydrodynamics, two-phase flow, CFD, level-set, large-scale simulation, moving contact line.

1 Introduction

Flows with moving contact lines involve a large range of length scales, from the nanometrical scale wherein some slip is usually considered to circumvent a singularity in the viscous stress [1], up to a larger (macroscopic) scale, that we want to be able to simulate. Resolving the flow down to the smallest scale (Direct Numerical Simulation) is not feasible for practical applications due to the disparity in length scales involved [2]. We thus resort to large-scale simulation, wherein the flow is resolved down to an intermediate scale, and the under-resolved part of the fow is represented using a hydrodynamic model (Cox's [3, 4] here).

2 Numerical method

We make use here of a one-fluid formulation: we solve for one set of Navier-Stokes equations (momentum equation and conservation of mass, with appropriate boundary conditions) and use the level-set function ϕ for interface-capturing (chosen as the signed distance to the interface); a standard advection

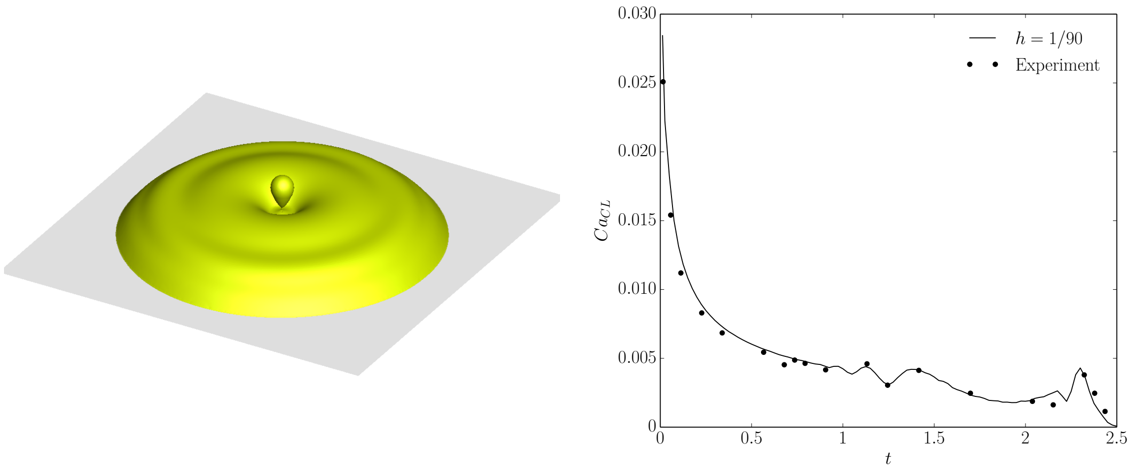

Figure 1: (a) Axisymmetric droplet spreading (simulated in 3D) in inertial leading to ejection of a small droplet (at $t = 2.15$), which is consistent with the experiment [8]. (b) Time signal of the contact line speed.

equation is used to advance the level-set function. Several level-set methods for spatial and temporal discretization have been tested and validated on several benchmark tests [5] (with or without the Navier-Stokes solver). The level-set code was developed further to account for contact line dynamics in three-dimensional flows with moving contact lines [6]. The method basically consists in enforcing the contact line speed that is consistent with the interface slope in the intermediate region (known from Cox's theory), which is the smallest scale resolved in the numerical simulation.

3 Some results

First series of validation tests were conducted against axisymmetric droplet spreading, with comparison to DNS results [7] for viscous spreading and experimental results [8] for inertial spreading. Very good qualitative and quantitative agreement was observed for these two axisymmetric cases, both simulated in 3D. In particular, a new regime of droplet ejection observed in [8] could be simulated using the CFD methodology developed here (Figure 1a). Quantitatively, the spreading rate compares very well with the experiment: in Figure 1b, for instance, the time signal of the contact line speed exhibits a local maximum at $t \simeq 2.3$, corresponding to a capillary wave arriving a the contact line, which is consistent with the experiment.

The code was then tested for 3D viscous drops sliding down an inclined planar homogeneous substrate. Results were in good qualitative agreement with prior experiments [9, 10]. Specifically, oval drops, cornered drops and pearling drops (Figure 2a) were observed, as in the experiment – pearling drops may appear by increasing the inclination angle of the substrate, leading to stretching of the drop and further to a capillary instability. Quantitative comparisons were also conducted for the drop geometry and sliding speeds. Convergence tests for the oval drop regime are presented in Figure 3; results are nearly independent on the grid spacing. Results for the speed in the pearling regime are also in satisfactory agreement with the experiment (Figure 2b).

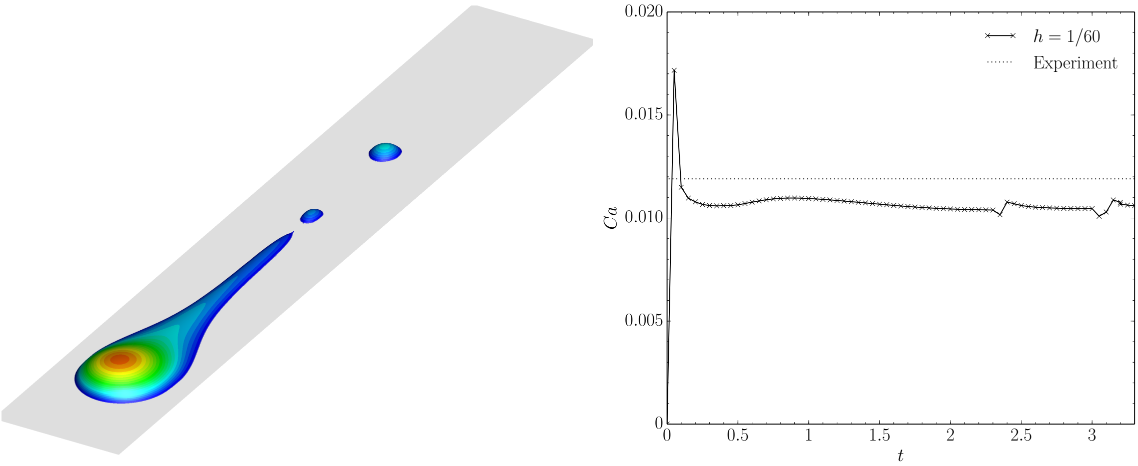

Figure 2: (a) Pearling drop observed in numerical simulation, which is consistent with the experiment [9]. The inclination parameter is $Bo \sin \alpha = 1.69$, with Bo the Bond number and α the inclination angle. The interface is colored by the height. (b) Time signal of the contact line speed.

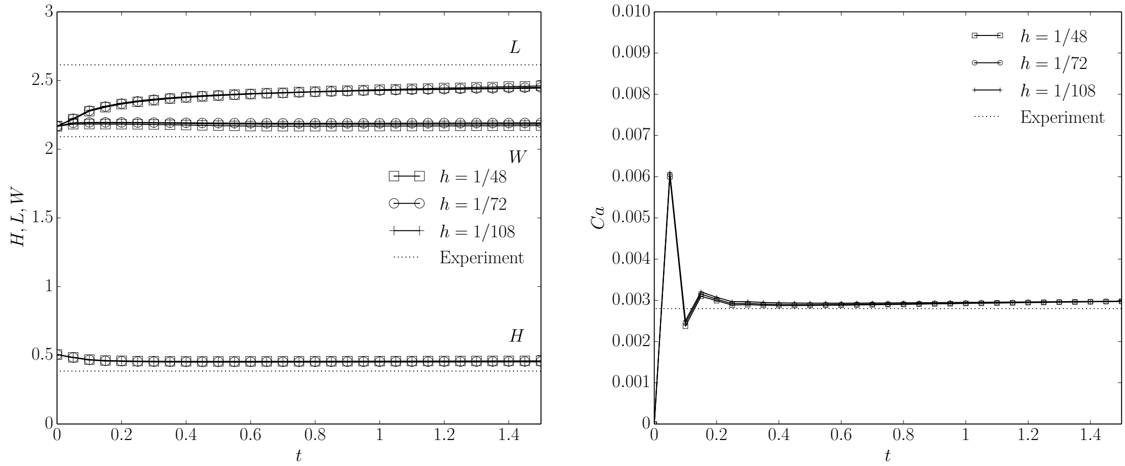

Figure 3: Results of convergence tests conducted for the oval drop regime, with comparison to experiment of [10]. The inclination parameter is $Bo \sin \alpha = 0.65$.

4 Conclusions

A CFD methodology has been developed for the numerical simulation of 3D flows with moving contact lines. Validation tests for axisymmetric spreading in the viscous regime or in the inertial regime are in very good agreement with prior work, as well as 3D tests in the viscous regime. It is thought that the CFD methodology may be applied to consider further complexities such as heterogeneous substrates, Marangoni stresses [11], providing that appropriate models are developed.

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