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Numerical method for three-dimensional macroscale simulations of two-phase flows with moving contact lines

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Résumé :

Un modèle d'angle de contact dynamique est développé avec une méthode level-set pour simuler des écoulements macroscopiques tridimensionnels avec lignes de contact mobiles. Le code est validé à partir de simulations numériques directes et résultats expérimentaux d'étalement de gouttelette en régimes visqueux et inertiel. Le code permet de simuler des écoulements tridimensionnels avec ligne de contact mobile en tenant compte de l'hystérésis de l'angle de contact.

Abstract:

A dynamic contact angle model is developed with a level-set method to simulate three-dimensional macroscopic flows with moving contact lines. The code has been validated against Direct Numerical Simulations (DNS) and experimental results of droplet spreading in viscous and inertial regimes. The code allows simulating three-dimensional flows with moving contact lines taking into account contact angle hysteresis.

Key words: hydrodynamics, two-phase flow, free surfaces and interfaces, CFD, macroscale simulation, moving contact line.

1 Introduction

A straightforward way to simulate a macroscopic flow involving contact line motion is to impose a constant contact angle value as boundary condition, equal to the static angle. Another trend is to use a relationship that links the contact angle and the contact line velocity. The latter is often preferred in studies of droplet dynamics, thin films flows and wetting phenomena [1]. In either case, numerical simulation for such flows under experimental conditions would require resolving the flow near a moving contact line down to a length scale that governs the contact-line motion [1-3], which is typically of the order of 10^{-8} meters, which is not practical. A level-set method [4] has been previously extended to account for a macroscale model that circumvents having to resolve the flow locally on a very small length scale, and that is based on asymptotic theory, but only for two-dimensional and axisymmetric flows [5]. Here, a new method is developed for fully three-dimensional level-set simulations with moving contact lines based on Cox's model [3], equally based on asymptotic theory. For instance, in viscous regime with small viscosity ratio μ_G/μ_L, Cox's theory [3] allows writing the interface slope θ at a distance d to an advancing contact line as a function of the wall angle θ_w, the capillary number Ca_{CL} based on the contact line speed, the slip length λ and a parameter Q that depends both on θ_w and the slip law that is used:

$$\theta^3 = \theta_w^3 + 9Ca_{CL}\left(\ln\left(\frac{d}{\lambda}\right) + Q\right) + O(Ca_{CL}^2) \quad (1)$$

Such a model is necessary for performing large scale simulations of moving contact lines, especially in three dimensions.

2 Numerical method

A pre-existing, well-tested two-phase flow solver based on a level-set method, TPLS [6], has been generalized for the simulation of flows with moving contact lines using a macroscale model. A level-set method [4] allows simulating two-phase flows with evolving interfaces with a one-fluid model. The level-set function is defined as the signed distance to the interface so that the zero level-set locates an interface. As the interface moves with the fluid, the evolution of the level-set function is given by an advection equation. That advection step introduces numerical errors and the level-set function φ may not remain a distance function thereafter. The condition $|\nabla\varphi| = 1$ should then be enforced so the level-set function is still a distance function. The Hamilton-Jacobi equation can be solved iteratively to maintain a distance function:

$$\frac{\partial\varphi}{\partial\tau} + \mathrm{sgn}(\varphi)(|\nabla\varphi| - 1) = 0 \quad (2)$$

Equation (2) is discretized using an upwinding procedure so that information propagates away from the interface. Therefore, there is always some information missing on one side of the contact line: that side is called the blind spot [7]. The main issue of flows with moving contact lines is to populate the level-set field in the blind spot avoiding numerical instabilities when solving Equation (2). In their axisymmetric simulations, Sui & Spelt [5] calculated the contact line speed and populated the blind spot so the interface slope at the wall boundary respects the dynamic contact angle model. Here, in three dimensions, the blind spot is populated so that the boundary angle θ, at a normal distance from the wall $z = \Delta z/2$, calculated with the level-set function $\cos\theta = -\partial\varphi_z/|\nabla\varphi|$, and the contact line speed respect the dynamic contact angle model of Equation (1) while avoiding numerical instabilities that may arise when solving Equation (2). Such an efficient model is needed for performing large scale simulations of moving contact lines, especially in three dimensions.

3 Validation tests

The three-dimensional code is validated for axisymmetric droplet spreading in viscous regime against Direct Numerical Simulation (DNS) (obtained in [8]) and compared with corresponding axisymmetric macroscale simulations of Sui & Spelt [5] wherein the flow on the entire range of length scales is resolved. Figure 1 shows that converged three-dimensional results in terms of spreading radius and contact line speed compare very well with both converged axisymmetric results obtained with Cox's model and DNS results all available in [5]. Validation tests have also been performed against the experiment of Ding et al. [9] that is axisymmetric droplet spreading in inertial regime, for which the relationship between the boundary angle and the contact line speed has been previously modified [3,5]. Fully three-dimensional flows with moving contact lines have also been simulated taking into account contact angle hysteresis.

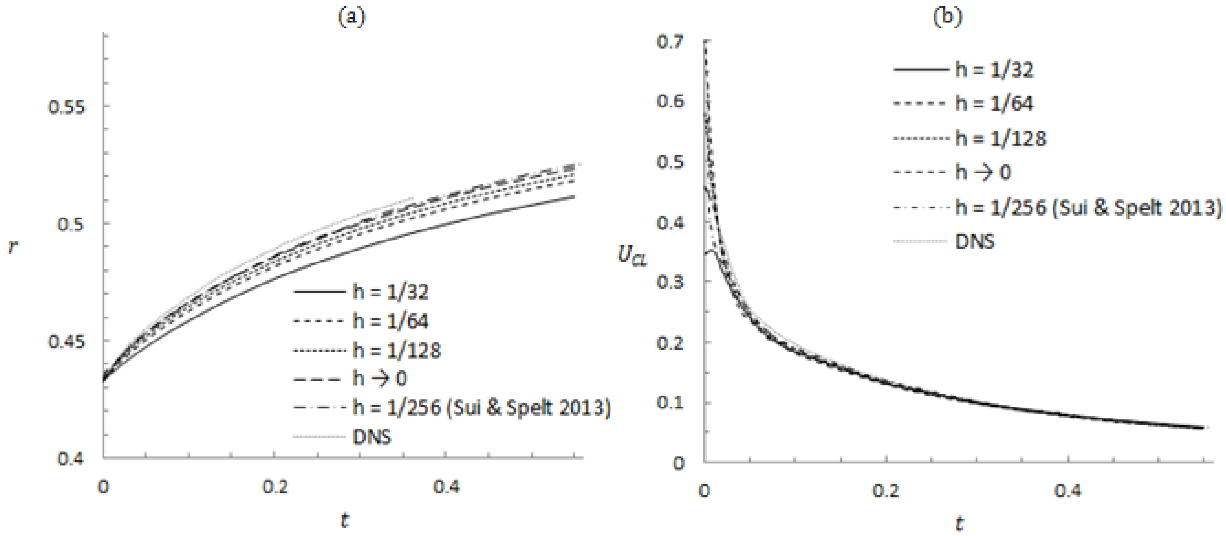

Figure 1. Validation against DNS and results of Sui & Spelt [5] for axisymmetric droplet spreading in viscous regime in terms of spreading radius (a) and contact line speed (b).

4 Conclusions

A new computational method is developed with a level-set method to perform macroscale simulations of flows with moving contact lines. The model has been validated against axisymmetric cases in viscous and inertial regimes and fully three-dimensional flows with contact angle hysteresis.

The authors gratefully acknowledge IFP Energies nouvelles for financial support, and the méso-centre FLMSN for the use of the computational resources. The authors gratefully acknowledge Lennon Ó Náraigh of University College Dublin for providing the original TPLS code and for further discussions, as well as Yi Sui of Queen Mary University of London for fruitful discussions.

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