Computers & Fluids 113 (2015) 2–13

Contents lists available at ScienceDirect

Computers & Fluids

journal homepage: www.elsevier.com/locate/compfluid

Comparison between numerical models for the simulation of moving contact lines

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ARTICLE INFO

Article history:
Received 11 December 2013
Received in revised form 30 June 2014
Accepted 8 September 2014
Available online 16 September 2014

Keywords:
Moving contact line
Numerical model
Spreading drop

ABSTRACT

The aim of this study is to discus different numerically models for the simulation of moving contact lines in the context of a Volume of Fluid–Continuum Surface Force (VoF–CSF) method. We focus on the particular situation of spreading drops. We first present the numerical methods used for the simulation of moving contact line i.e. static contact angle versus dynamic contact angle, no slip condition versus slip condition. A grid and time convergence is performed for the different models. We show that the integration of the Continuum Surface Force using the finite volume method results in a grid dependence at the onset of the spreading. The static and dynamic models are compared to experiments. It is shown that the dynamic models based on the Cox's relation for the dynamic contact angle are able to reproduce experiments while static models overestimate the spreading time and are not able to reproduce the Tanner regime. The difference between static and dynamic models is shown to increase with the Ohnesorge number.

1. Introduction

The numerical methods developed for the simulation of moving contact line differ by: (i) the type of the numerical methods used to describe and transport the interface, (ii) the wall boundary condition imposed for the description of the contact line. For the transport of the interface, we give here some examples showing that almost all the classical methods are concerned: Boundary Integral methods [1–3], adaptive grid methods [4,5], Level-Set methods [6,7], Volume of Fluid methods [8–10], Front Tracking Methods [11,12] and coupled Level set and Volume-of-Fluid (CLSVOF) methods [13]. Different methods have also been developed for the modeling of moving contact lines. Most of the methods are able to impose a given contact angle θ_W made by the interface at the contact line. The condition is applied to the normal made by the interface at the wall. The simplest situation is then to impose a constant angle corresponding to the static angle, i.e. $\theta_W = \theta_S$ [8,11,7,6,9]. When a no-slip condition is imposed on the wall, the stress generated by a contact line moving at velocity U_{cl}, can be estimated as

$$\tau_{xy} \approx \mu \frac{U_{cl}}{\Delta} \quad (1)$$

where Δ is the grid spacing and μ is the fluid viscosity. The stress at the contact line is clearly diverging when refining the grid size (see for example [14] where the evolution of the viscous stress at the wall is reported). Several authors [8,6,14] have dealt with the "stress singularity" paradox by introducing the Navier slip condition that gives a relation between the fluid velocity at the wall U_W and a Navier slip length λ_N:

$$U_W = \lambda_N \frac{\partial U}{\partial n_W} \quad (2)$$

where n_W is the normal to the wall. The grid convergence is then obtained by solving the full hydrodynamic problem inside the hydrodynamics slip region. Unfortunately, due to the grid refinement limitation, most of these simulations use unrealistically large slip length values and therefore the Navier slip length λ_N becomes in practice an adjustable parameter for the simulation (see Bonn et al. [15]). The grid convergence of the simulations is then reached but an unphysical slip condition is necessary. In recent developments, the dynamic or apparent contact angle is connected to the velocity of the contact line. The Cox [16] relation is directly applied [10,17] or adapted using an adjustable parameter that needs to be empirically determined from experiments [13,14].

As shown in this introduction, different strategies have been developed for the simulation of moving contact line. We discuss and compare different possible modelings in the first part of this paper. Then the numerical models are compared with experiments of spreading drop.

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http://dx.doi.org/10.1016/j.compfluid.2014.09.018
0045-7930/

2. Numerical method

2.1. VoF solver

The numerical simulations reported in this work are performed with the Volume of Fluid (VoF) solver developed in the JADIM code [18,10]. The one-fluid system of equation is obtained by introducing the one-fluid function C used to localize one of the two phases. In this study, we define C as $C = 1$ in the liquid, here the drop, and $C = 0$ in the external fluid. The one-fluid function C makes possible the definition of the one fluid variables $U = CU_1 + (1-C)U_2$ for the velocity, $P = CP_1 + (1-C)P_2$ for the pressure, $\rho = C\rho_1 + (1-C)\rho_2$ for the density and $\mu = C\mu_1 + (1-C)\mu_2$ for the viscosity. The position of the interface is then given by the transport equation:

$$\frac{\partial C}{\partial t} + U \cdot \nabla C = 0 \tag{3}$$

The two fluids are assumed to be Newtonian and incompressible with no phase change. Under isothermal condition and in the absence of any surfactant the surface tension is constant and uniform at the interface between the two fluids. In such condition, the velocity field U and the pressure P satisfy the classical one-fluid formulation of the Navier–Stokes equations:

$$\nabla \cdot U = 0 \tag{4}$$

$$\rho\left(\frac{\partial U}{\partial t} + U \cdot \nabla U\right) = -\nabla P + \nabla \cdot \Sigma + \rho g + F_\sigma \tag{5}$$

where Σ is the viscous stress tensor, g is the gravity and F_σ is the capillary contribution:

$$F_\sigma = \sigma \nabla \cdot n\, n \delta_I \tag{6}$$

where σ is the surface tension, n denotes by arbitrary choice the unit normal of the interface going out from the drop and δ_I is the Dirac distribution associated to the interface.

The system of Eqs. (3)–(6) is discretized using the finite volume method. Time advancement is achieved through a third-order Runge–Kutta method for the viscous stress. Incompressibility is satisfied at the end of each time step though a projection method. The overall algorithm is second-order accurate in both time and space. The volume fraction C and the pressure P are volume-centred and the velocity components are face-centred. Due to the discretization of C, it results a numerical thickness of the interface, cells cut by the interface corresponding to $0 < C < 1$. The interface location and stiffness are both controlled by an accurate transport algorithm based on FCT (Flux-Corrected-Transport) schemes [19]. This method leads to an interface thickness of about three grid cells by the implementation of a specific procedure for the velocity used to transport C in flow region of strong strain and shear [18]. The interfacial force is solved using the classical CSF (Continuum Surface Force) model [20]:

$$F_\sigma = \sigma \nabla \cdot \left(\frac{\nabla C}{|\nabla C|}\right) \nabla C \tag{7}$$

The induced spurious currents have been characterized [10] and their maximum magnitude evolve as $0.004\sigma/\mu$, in agreement with other codes using the Brackbill's formulation.

2.2. Numerical modeling of the contact angle

The numerical method for the simulation of static and dynamic contact angles has been developed by Dupont and Legendre [10] for 2D and axisymmetric geometries, and recently extended to 3D geometries [21]. The calculation of the capillary term requires the knowledge of the value of the contact angle made by the interface at the wall. Indeed, the capillary contribution in the momentum Eq. (6) requires the knowledge of ∇C. Furthermore, $\nabla C/|\nabla C|$ being the normal of the interface, the boundary condition for ∇C is thus directly given by the value of the contact angle θ_W by the following relation:

$$\frac{\nabla C}{|\nabla C|} = n = \sin\theta_W\, n_\parallel + \cos\theta_W\, n_\perp \tag{8}$$

where the unit vectors $n_\parallel$ and $n_\perp$ are the components of the normal vector n, parallel and normal to the wall, respectively. The general method is decomposed into two steps. We first determine the value of the contact angle to apply at the wall. This value is then imposed as a boundary condition using relation (8) for the calculation of the capillary contribution (7) in the momentum balance (5). One objective of this work is to compare different possible modeling to the dynamic modeling introduced in our code JADIM (model Dyn2 in the following). The tested models are reported in Table 1. The two main parameters that characterize these models are the description of the contact angle $\theta_W(t)$ and the description of the fluid boundary condition. The Navier slip condition (1) can be imposed in order to remove the stress singularity at the contact line with the introduction of the Navier slip length λ_N. If $\lambda_N = 0$ a classical no-slip condition is imposed. When considering ordinary fluids and wall properties, a relevant value for the slip length is $\lambda_N = O(10^{-9})$ m [22]. Note that imposing such slip lengths for solving millimeter size drop with 100 regular cells per radius ($\Delta \sim R/100 \sim 10^{-5}$ m) which is a very accurate description of the macroscopic flow field is equivalent to impose a no-slip condition. In the following we consider two sorts of model: "static" models (Stat1, Stat2 and Stat3) and "dynamic" models (Dyn1, Dyn2, Dyn3 and Dyn4). The simplest model, called "Stat1", consists in imposing the contact angle constant as the Young value θ_S with no slip condition $\lambda_N = 0$. When imposing a constant contact angle $\theta_W(t) = \theta_S$, the effect of the sliding condition (1) has been examined by imposing a slip length linked to the grid size $\lambda_N = \Delta/2$ (model "Stat2") as suggested by Afkhami et al. [14] or a fixed value for the slip length $\lambda_N = \Delta_{32}/2$ (model "Stat3") where Δ_{32} is the grid spacing corresponding to 32 regular cells per radius which is the coarser grid used in this study (see next section for the description of the numerical parameters). The dynamic models are expressed as a function of the contact line Capillary number Ca defined as

$$\mathrm{Ca} = \frac{\mu_1 U_{cl}}{\sigma} \tag{9}$$

where U_{cl} is the contact line velocity. In our VoF formulation, U_{cl} is the interface velocity interpolated at $C = 0.5$. Due to the staggered grid structure, U_{cl} is located at the distance $\Delta/2$ from the wall where the node of the tangential component of the velocity that transports the interface is located. We have first tested the model (called "Dyn4") proposed by Afkhami et al. [14]. Based on 2D simulations and the expression developed by Cox [16], they proposed the following expression for the dynamic contact angle

$$\cos\theta_d = \cos\theta_S + 5.63\mathrm{Ca}\log\left(\frac{K}{\Delta/2}\right) \tag{10}$$

The simulations reported by Afkhami et al. [14] show that it ensures grid convergence in VoF simulations when coupled with a slip length based on the grid spacing $\lambda_N = \Delta/2$. The authors suggest that "the true value of K could be determined by fitting numerical data to data obtained experimentally". In their simulations, a constant value $K = 0.2L$ is proposed for a plate withdrawing from a square fluid pool of length L while the authors use $K = 0.04R$ for their simulations of the spreading of droplet of initial radius R. This smaller value of K was chosen because their model is only valid for $|\cos\theta_d| < 0.6$. The model "Dyn1" corresponds to the original model implemented in JADIM by Dupont and Legendre [10]. The dynamic