An original algorithm for VOF based method to handle wetting effect in multiphase flow simulation

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ARTICLE INFO

ABSTRACT

The numerical modeling of contact angle and wetting surface properties is investigated with volume of fluid (VOF) interface tracking method. A method is proposed to model the wetting properties with an existing continuum surface force (CSF) approach by introducing an original smooth volume of fluid function (SVOF) resulting from the solving of a penalized Helmholtz equation. For the diffusion equation proposed here, the interest of the penalty method is to account implicitly for wetting effects and, to avoid introducing sliding laws for the velocities at the wall or modifying by hand the interface shape on the solid boundaries. The SVOF model is validated and evaluated on published experiments concerning droplet impacts on flat and inclined surfaces with various wetting properties.

Published by Elsevier Ltd.

1. Introduction

The numerical simulation of two-phase flows involving wetting effects is of interest for numerous fundamental and applied researches in fluid mechanics applied to material selection, surface treatment, heat exchangers, energy production or lubrication in industrial processes. The unsteadiness and complex optical properties of two-phase flows make the experimental measurements difficult to achieve and have encouraged research efforts to build efficient physical models and numerical methods.

Among the wide variety of physical approaches, two main fundamental modeling strategies exist, based on microscopic considerations or continuous fluid mechanics. Molecular dynamics of multiphase flows involve molecular interfacial forces [1,2], which act on a smaller scale than the minimum numerically resolved structures and are responsible for an interface energy excess. Microscopic models integrate molecular forces into continuous models. These latter models introduce diffuse interfaces and contain a complete description of capillary effects – including wetting-through thermodynamically consistent equations. The resolution of diffuse interfaces can only be applied to problems involving small ranges of interfacial scales to keep reasonable computational grids in three dimensions.

The models based on continuous fluid mechanics are the most commonly used in academic and industrial CFD tools. They are built by integrating the Navier–Stokes equations in each phase and by defining jump relations at the interface to ensure mass and momentum conservation [3]. Considering fixed structured grids, the interface is not explicitly discretized on the mesh used to solve the Navier–Stokes equations. Kataoka [4] introduce a phase function variable C to define the local volume fraction in each grid cell. The Navier–Stokes equations in each phase are generalized to the whole two-phase medium by convolving the conservation equation by C and integrating them among all the control volumes. Finally, a single fluid model, also called 1-fluid model, is obtained, which contains a new force in the momentum equations accounting for the surface tension effects. This single fluid model requires the solving of an advection equation on C to describe the time and space evolutions of the interface. A wide variety of methods have been proposed over the last 20 years to numerically treat the advection of C, such as the Front Tracking method [5], the level set technique [6], or the volume of fluid (VOF) approach [7]. We choose to use the single fluid model and to improve VOF methods to simulate wetting effects as these approaches are among the most popular in the field of two-phase flow simulation. In the VOF methods, the surface tension force is classically approximated with the continuum surface force (CSF) of Brackbill et al. [8], which formulates the interfacial force as a function of the gradients of C. An extension of the CSF approach is proposed in this work to treat the dynamic contact angle in VOF methods. The reader can refer to the work of Manservisi and Scardovelli [9] for a review of two-phase flow models dedicated to contact angle on fixed grids.

First, the filtered 1-fluid model is presented briefly. An original extension of the CSF method, which uses an auxiliary diffuse VOF

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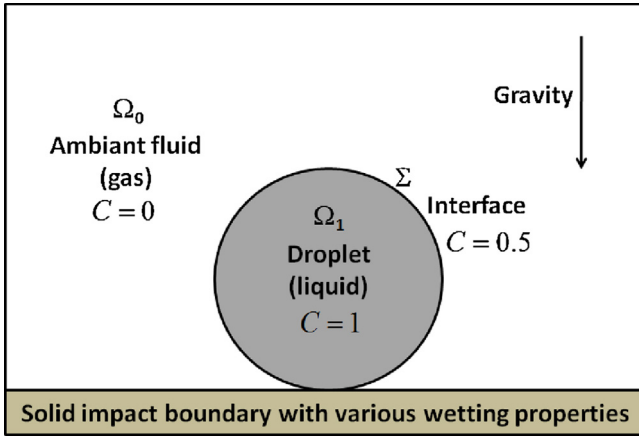 *E-mail address:* guillaument@icmcb-bordeaux.cnrs.fr (R. Guillaument).

Fig. 1. Definition sketch of the droplet impact on a solid boundary according to the fictitious domain approach.

variable, is then detailed and the numerical implementation of the single fluid CSF model for wetting effects is explained. Several test cases are done to show the advantages of this model. Then, the regularized CSF approach on the impact of a droplet on a dry surface for various wetting conditions is illustrated. These numerical tests are used to validate the physical meaning of the numerical model for wetting. Finally, concluding remarks are provided.

2. Two-phase model and numerical methods

2.1. The 1-fluid model

As previously explained, the modeling and the simulation of two-phase flows involving separated phases, i.e. the characteristic interfacial length scale is larger than the smallest spacing of the computational grid, is classically achieved by introducing the Navier–Stokes equations in each phase [10] and by insuring the connection of the velocity field at the interface by defining jump conditions on the velocity and the stress tensor [3]. Another point of view, chosen in this work, consists in defining a unified flow model valid in all phases and at the interface. This single fluid model of Kataoka [4], also called 1-fluid, is widely used to solve in problems involving three-dimensional problems and strong interface deformations. In this modeling framework, the two-phase flow representation is restricted to non miscible, incompressible and isothermal fluids. Moreover, a constant surface tension is assumed. The required jump equations valid at the interface [3] are directly integrated in the 1-fluid model by convolving the single phase conservation equations with a phase function C describing the interface evolutions over time through a material advection equation. As described in Fig. 1, this color function C is assumed to behave like a Heaviside function as the following:

$$C(x, t) = \begin{cases} 1 & \text{if} \quad x \in \text{phase} \quad k = 1 \\ 0 & \text{if} \quad x \in \text{phase} \quad k = 0 \end{cases} \tag{1}$$

The interface Σ between phases Ω_0, i.e. $C = 0$, and Ω_1, i.e. $C = 1$, is defined by the isosurface $C = 0.5$. Using the color function, local quantities such as the density ρ or the dynamic viscosity μ are, for example, defined by numerical mixture laws such as:

$$\begin{aligned} \rho &= C\rho_1 + (1 - C)\rho_0 \\ \mu &= C\mu_1 + (1 - C)\mu_0 \end{aligned} \tag{2}$$

With respect to these definitions, a single set of Navier–Stokes equations for a two-phase flow is designed in the framework of the 1-fluid formation [4,10]:

$$\rho \left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) = -\nabla p + \rho \mathbf{g} + \nabla \cdot (\mu [\nabla \mathbf{u} + \nabla^T \mathbf{u}]) + \mathbf{F}_{ST} \tag{3}$$

$$\nabla \cdot \mathbf{u} = 0 \tag{4}$$

$$\frac{\partial C}{\partial t} + \mathbf{u} \cdot \nabla C = 0 \tag{5}$$

where $\mathbf{F}_{ST}$ is the surface tension force depending on the interface location. This force is modeled by a continuum surface force (CSF) approach based on the work of Brackbill et al. [8]:

$$\mathbf{F}_{ST}(C) = \sigma \kappa \mathbf{n} \delta_i = \sigma \nabla \cdot \left(\frac{\nabla C}{\|\nabla C\|} \right) \nabla C \tag{6}$$

The notation κ denotes the local mean curvature of the interface, σ the constant surface tension coefficient, $\mathbf{n}$ the normal to the interface and δ_i the Dirac function indicating the interface. The single-field representation of the flow (3)–(5)) relies on several assumptions. First, the advection Eq. (5) on phase function C describes the topological modifications of the interface without phase change. Through this equation, the color function C is advected with the local fluid velocity $\mathbf{u}$ and consequently, the evolution of both phases (fluid 0 and 1) is known at each physical time and at each position in the calculation domain. The single velocity field of the interfacial flow is incompressible, i.e. $\nabla \cdot \mathbf{u} = 0$ through Eq. (4), due to the fact that each phase is incompressible and no sliding between the phases occurs on a macroscopic point of view [11].

2.2. A smooth boundary interface model for modeling capillary effects

One of the main limitations of recent VOF methods is associated with the generation of artificial deformations of the interface, and the creation of small artificial blobs [12–17] when the characteristic length-scale of interfaces is comparable to the local grid size. Moreover, if we refer to the modeling of the surface tension term (6), then the discretization of the surface tension force and in particular the obtention of a curvature estimate requires the approximation of second order partial derivatives of the VOF function, whose gradients are restricted to one numerical control volume. As a consequence, the compact support of the discrete surface tension force, relying on centered schemes following the work of Brackbill [8], is incomplete, as the VOF function only varies on one cell. Our main idea is to build an auxiliary Smooth VOF (SVOF) function called C^S, which will be obtained thanks to C, in order to estimate the curvature and the normal to the interface required in Eq. (6). The use of additional functions the surface tension force has been proposed by Popinet [18] and Gueyffier [19], who introduces height functions and analytical curvature estimates in order to calculate on a discrete level the local interface curvature.

The building of a smooth color function was also proposed by Rudman [20] who implemented the Kernel functions and applied the surface tension force formulation to the smooth C variable. The main difference between the various smooth function approaches previously proposed and our Smooth-VOF technique, is that our approach is consistent with the spreading of the phase function in the normal direction of the interface.

The smooth VOF will not explicitly replace the sharp VOF function C, in order to keep the correct mass conservation properties brought by the PLIC numerical algorithm [21] used in this work. The SVOF function is a post-treatment of C which should match the interface position, i.e. the position M such as $C(M) = 0.5$ is verified in