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3D numerical study of large-scale two-phase flows with contact lines and application to drop detachment from a horizontal fiber

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ABSTRACT

One fundamental problem in understanding two-phase flows in coalescers is determining how large of a drop can attach to and subsequently remain on a fiber. Droplet detachment can be caused by gravity or shear from the cross-flow overcoming the adhesion between the drop and the fiber. Previous studies have found the critical size of a drop on a hydrophilic fiber under gravity and the critical size of a drop on a hydrophobic fiber. In this paper, we present an accurate, conservative, and robust numerical strategy to simulate large-scale two-phase flows in complex geometries, and validate the capability of the proposed approach to predict the critical size of a drop on a cylindrical hydrophilic fiber under gravity and on a hydrophobic fiber without gravity. Then, an exploratory study of the critical size of a drop on a cylindrical fiber with cross-flow is performed.

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1. Introduction

Two-phase flows with moving contact lines are ubiquitous in many natural and industrial applications. This includes ink-jet printing, internal combustion engines (Yarin, 2006), micro-fluidics applications (Darhuber and Troian, 2005), and two-phase flows in porous media (Zinchenko and Davis, 2017), to name a few. In this work, we numerically study two-phase flows in a common industrial equipment, namely a coalescer. Coalescers are filters made from fibrous materials that collect fine droplets dispersed in a continuous phase. In industry, fiber-based coalescers are used to separate two immiscible fluids. For example, coalescers are used to recover liquid water from morning fog in desert areas, and coalescers can be employed to mitigate noxious aerosol emission from chemical plants. However, if the concentration of liquid within the coalescer becomes too large, the coalescer become saturated and the gas stream can re-atomize the coalesced liquid into small droplets. In order to mitigate saturation and optimize the performance of a liquid–gas coalescer, a detailed understanding of the multiphase flow inside coalescers is necessary. Unfortunately, direct experimental observation is not easy to achieve inside a coalescer, because fibers are not made of transparent materials, and they are irregularly arranged. Lorenceau et al. (2004) started with droplets interacting with a single fiber. To better describe several drops passing by a single fiber, we divide the process into three conceptual stages: capture, accumulation, and detachment. Here, capture refers to droplets hitting a fiber and staying on the fiber, accumulation refers to the coalescence of droplets with droplets already captured on the fiber to form larger droplets, and detachment refers to captured droplets leaving a fiber. In this work, we numerically study the last stage of the process, drop detachment from a single fiber, to provide some insight into the fundamental physics which can be used in future design.

A computational strategy based on recently developed methods (Desjardins et al., 2008; Luo et al., 2016; Meyer et al., 2010) is employed in this work to study two-phase flow in complex geometries. This strategy utilizes a conservative level-set method to capture the liquid gas interface (Desjardins et al., 2008; Olsson and Kreiss, 2005; Olsson et al., 2007). In the level-set approach, the interface is defined implicitly as an iso-surface of a smooth function. There are many benefits of this approach, such as automatic handling of topology changes and efficient parallelization. In the conservative level-set approach, the auxiliary function is a hyperbolic tangent function, which improves mass conservation, but makes the calculation of normals and curvature more challenging. Improved with a newly-developed reinitialization strategy (Chiodi and Desjardins, 2016), the Accurate Conservative Level-Set (ACLS) method is capable of simulating liquid–gas flows with complex interface deformation in 3D with large density ratios (Desjardins et al., 2013).

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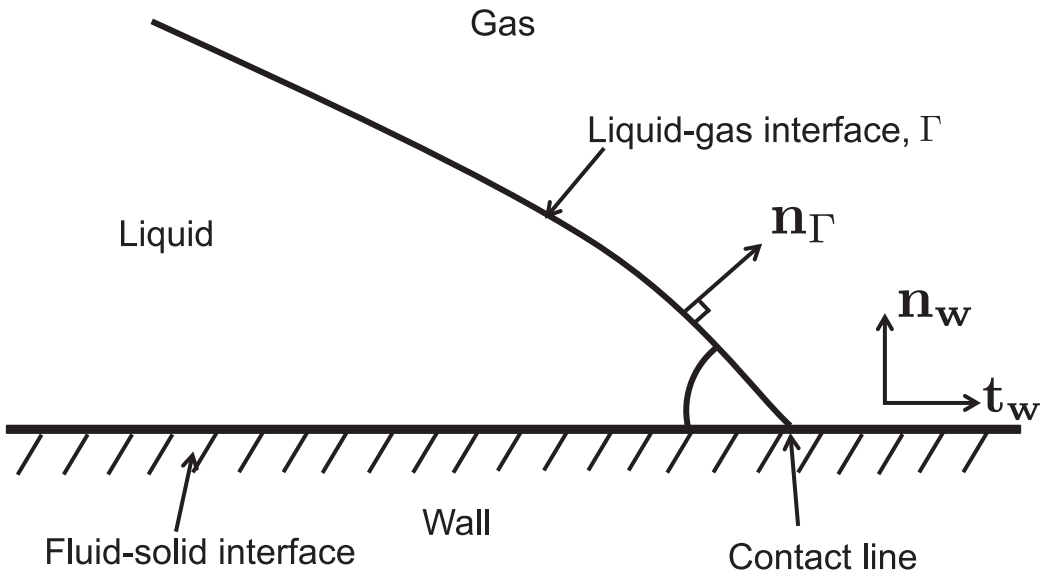

Fig. 1. Schematic of the triple-phase area near the contact line.

A conservative immersed boundary method based on the cut-cell approach of Meyer et al. (2010) is employed to represent the solid phase (Desjardins et al., 2013). The cut-cell methodology provides a sharp immersed boundary representation and conserves mass and momentum discretely.

One approach to impose the contact angle is to resolve all regions of the flow using molecular dynamics simulations. However, molecular dynamics simulations are restricted to very small systems and very simple model fluids (Sui et al., 2014). Therefore a model at the scale of a single drop is preferred. The contact line model in this work is a curvature boundary condition method originally proposed by Luo et al. (2016), which allows to implicitly impose the contact angle of the liquid–gas interface. This method has less spurious level-set displacement and less mass conservation error (Luo et al., 2016). In this work, a strategy is proposed to extend the curvature boundary method to 3D on curved boundaries.

The outline of this paper is as follows: The mathematical formulation is presented in Section 2, followed by details of the implemented conservative level-set method, the conservative immersed boundary method, and the curvature boundary method in Section 3. In Section 4, we test the accuracy, conservation, and robustness of proposed method via three test cases. Finally, droplet detachment from a fiber is explored in Section 5.

2. Mathematical description

As shown in Fig. 1, the problem of interest includes three phases, i.e., liquid phase, gas phase, and solid phase, and three interfaces, i.e., liquid–gas interface, liquid–solid interface, and gas–solid interface, all three converging at the contact line. For liquid and gas phases, the governing equations considered are the incompressible Navier–Stokes equations. The solid phase does not move nor deform in the scope of this study, thus there is no need to represent its dynamics. The mathematical description for the fluid and the interfaces is provided below.

2.1. Liquid and gas phases - incompressible Navier-Stokes equations

The multiphase flow of interest in this work occurs at low Mach numbers, therefore we use the incompressible form of the Navier–Stokes equations, which is written as

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla(\rho \mathbf{u} \otimes \mathbf{u}) = -\nabla p + \nabla \cdot \left(\mu\left[\nabla \mathbf{u} + \nabla \mathbf{u}^{\mathsf{T}}\right]\right) + \rho \mathbf{g}, \tag{1}$$

where $\mathbf{u}$ is the velocity field, p is the pressure, ρ is the density, μ is the dynamic viscosity, and $\mathbf{g}$ is the gravitational acceleration. The continuity equation with the incompressible constraint is written as

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = \frac{\partial \rho}{\partial t} + \mathbf{u} \cdot \nabla \rho = 0. \tag{2}$$

Note that the material properties of both phases are taken to be constant, thus in the liquid phase, $\rho = \rho_l$ and $\mu = \mu_l$, and in the gas phase, $\rho = \rho_g$ and $\mu = \mu_g$.

2.2. Liquid–gas interface

There is an interface Γ between the liquid and gas phases, and we use $[\rho]_\Gamma = \rho_l - \rho_g$ and $[\mu]_\Gamma = \mu_l - \mu_g$ to represent the jump in density and viscosity. The velocity field is continuous across the interface, thus $[\mathbf{u}]_\Gamma = 0$. The surface tension and the jump in viscous stresses combine to cause a pressure jump across the interface,

$$[p]_\Gamma = \sigma\kappa + 2[\mu]_\Gamma \mathbf{n}_\Gamma^{\mathsf{T}} \cdot \nabla \mathbf{u} \cdot \mathbf{n}_\Gamma, \tag{3}$$

where σ is the surface tension coefficient, κ is the interface curvature, and $\mathbf{n}_\Gamma$ is the liquid–gas interface normal.

2.3. Fluid–solid interface

At the fluid–solid interface the no-slip and impermeable boundary conditions are applied in this work. Thus, the normal velocity $\mathbf{u}_\perp = (\mathbf{u} \cdot \mathbf{n_w})\mathbf{n_w}$ and the tangential velocity $\mathbf{u}_\parallel = \mathbf{u} - \mathbf{u}_\perp$ are zero at the wall.

2.4. Contact line

The Young–Laplace equation determines the shape of a liquid–gas interface. The static contact angle (or equilibrium contact angle) θ_s is determined from the solid–gas interfacial energy, σ, the solid–liquid interfacial energy, γ_{SL}, and the liquid–gas interfacial energy, γ_{LG}, by Young's equation,

$$\gamma_{SG} - \gamma_{SL} - \sigma \cos\theta_s = 0. \tag{4}$$

Instead of solving the Young–Laplace equation to obtain a static contact angle in this study, we directly provide a static contact angle in all the simulations. There is an issue with the boundary condition because the interface moves and thus no-slip is not appropriate. The singularity at the contact line caused by the use of a

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