Computers and Fluids 171 (2018) 103–121

Contents lists available at ScienceDirect

Computers and Fluids

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

Finite element setting for fluid flow simulations with natural enforcement of the triple junction equilibrium

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ARTICLE INFO

Article history:
Received 19 March 2018
Revised 2 June 2018
Accepted 11 June 2018

Keywords:
Stabilised finite elements
Mesh adaptation
Pressure enrichment
Surface operators
Surface tension
Laplace's law

ABSTRACT

Capillary phenomena are involved in many industrial processes, especially those dealing with composite manufacturing. However, their modelling is still challenging. Therefore, a finite element setting is proposed to better investigate this complex issue. The variational formulation of a liquid–air Stokes' system is established, while the solid substrate is described through boundary conditions. Expressing the weak form of Laplace's law over liquid–air, liquid–solid and air–solid interfaces, leads to a natural enforcement of the mechanical equilibrium over the wetting line, without imposing explicitly the contact-angle itself. The mechanical problem is discretised by using finite elements, linear both in velocity and pressure, stabilised with a variational multiscale method, including the possibility of enrichment of the pressure space. The moving interface is captured by a Level-Set methodology, combined with a mesh adaptation technique with respect to both pressure and level-set fields. Our methodology can simulate capillary-driven flows in 2D and 3D with the desired precision: droplet spreading, droplet coalescence, capillary rise. In each case, the equilibrium state expected in terms of velocity, pressure and contact angle is reached.

1. Introduction

Capillary phenomena are physical processes driven by the surface tension or surface energy of immiscible media [1–4]. The term "surface tension" is used when dealing with an interface between two fluids, while "surface energy" is employed when at least one of the domains in contact is a solid. For the sake of simplicity, these terms will be synonymously employed in this paper. However, there is still a fundamental difference between both of them: while surface tension refers to the stress state of the interface, surface energy refers to its energy density. In the situations investigated, three media, two fluids (liquid and gas) and a solid substrate, intersect at what is called a triple junction. This is a point, in two-dimensions, or a line, in three-dimensions, also called contact or wetting line. When in non-equilibrium, the force balance at the triple junction, causes the fluids to flow, and consequently induces a motion of the interface. This explains the spreading of a droplet on a solid substrate, as well as the rise of a liquid into a capillary tube, the two standard applications which will be discussed. Capillary phenomena have important implications in a wide range of industrial and scientific domains. For example, the fabrication of textured surfaces with superhydrophobic [5] properties, is still challenging for the automotive or aeronautics industry. In another context, the void formation observed in some bio-based composite materials, manufactured by liquid composite moulding, can be correlated to the value of the capillary number, that is the ratio between viscous and capillary forces [6,7].

Capillary phenomena will be described within a macroscopic continuum mechanics framework. In the literature dealing with computational aspects of capillary phenomena at continuum scale, the force balance at the triple junction is usually substituted for an angle condition to be enforced. Following the classification given by Sprittles and Shikhmurzaev [8], this enforcement is performed either essentially or naturally through the variational formulation. When the contact-angle condition is seen as an essential boundary condition, some iterative scheme is usually employed to alternatively compute the contact interface velocity and modify the geometry of the interface until reaching a steady state. This strategy is adopted by Bellet [9], Liu et al. [10], but also Spelt [11]. In this last reference, the geometry is modified in the reinitialisation step of the level-set interface-capturing method. The natural assignment of the contact-angle is based on the integration by part of the Laplace's law in the variational form of the mechanical problem. A boundary term, defined at the triple junction, appears when

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https://doi.org/10.1016/j.compfluid.2018.06.007
0045-7930/

integrating by parts. Then, it can be replaced by the angle condition in the variational problem, as described by Sprittles in [8,12]. Usually, this condition connects the apparent angle, static angle, and the flow in the vicinity of the triple junction. Mechanically, as mentioned by Buscaglia and Ausas [13], but also by different authors [14–16], the angle condition considers a localised dissipation which could model the roughness or heterogeneity of surfaces, for example.

This paper offers an original finite element model of wetting problems, based on a variational formulation of the mechanical problem, in which the force balance is naturally imposed at the triple junction. The two fluids, assumed to be Newtonian, represent a liquid and a surrounding medium (typically air). To simplify the computational complexity, inertia effects are neglected. Therefore, the mechanical problem is reduced to the bifluid Stokes' equations, which describe a quasi-static system, allowing only the transient evolution of the liquid-gas interface. Consequently, the objective of this paper is mainly to study the ability of the proposed approach to predict successfully the final steady equilibrium state, and not to capture the transient dynamics with accuracy.

A crucial point of our approach is to fully consider all three interfaces meeting at the triple junction. Hence, working out the balance of forces acting on a surface element leads directly to the weak formulation of Laplace's law. Subsequently, considering this on liquid, gas and solid interfaces, provides a variational formulation of the mechanical problem, which can deal with the surface energy discontinuity across the triple junction, as well as express implicitly the force balance at the triple junction. Contrary to most of the previous cited articles, this force balance is not described in contact-angle terms, but directly in terms of surface tension and surface energies. Consequently, the equilibrium value of the contact-angle is not imposed numerically, but results from the computation of this mechanical equilibrium at the triple junction. Computationally, the mechanical equations are discretised using a stabilised finite element (FE) technique. A level-set method, combined with an anisotropic mesh-adaptation strategy, is used to describe the moving interface with accuracy.

The rest of this paper is organised as follows. The mechanical problem, or bifluid Stokes' system, is presented and detailed in Section 2, with a special focus on the balance of forces acting on the interfaces and at the triple junction. Section 3 establishes the variational formulation of this system. In these two sections, a tensor analysis setting, based on the introduction of the co- and contra-variant tangent bases, is used to mathematically describe surfaces and their geometry. Using tensor analysis describes surfaces embedded in $\mathbb{R}^3$ and curves embedded in $\mathbb{R}^2$ in a unified framework. The computational strategy is detailed in Section 4. More precisely, the FE setting is given, including discrete problem stabilisation, pressure space enrichment, mesh adaptation strategy, and level-set method used to capture the interfaces. Finally, simulation results are shown in Section 5. First, accuracy of the FE framework is assessed through 2D-simulations of droplet spreading. Second, the numerical developments are used to carry out 3D-simulations of droplet spreading and flows in a capillary tube as well.

2. Mechanical problem

Let Ω be a bounded region of $\mathbb{R}^d$ ($d = 2, 3$ is the spatial dimension), also referred to as the computational domain. This domain contains two immiscible parts: a liquid part, denoted Ω_1, immersed in a surrounding medium Ω_2, also referred to as a gaseous medium or the air. Furthermore, the liquid Ω_1 is lying on a rigid substrate, identified with a boundary of the computational domain. Such a situation is illustrated for simplicity in 2D (Fig. 1): Ω is the unit square, while Ω_1 is half a liquid droplet spreading along the plane $\{y = 0\}$.

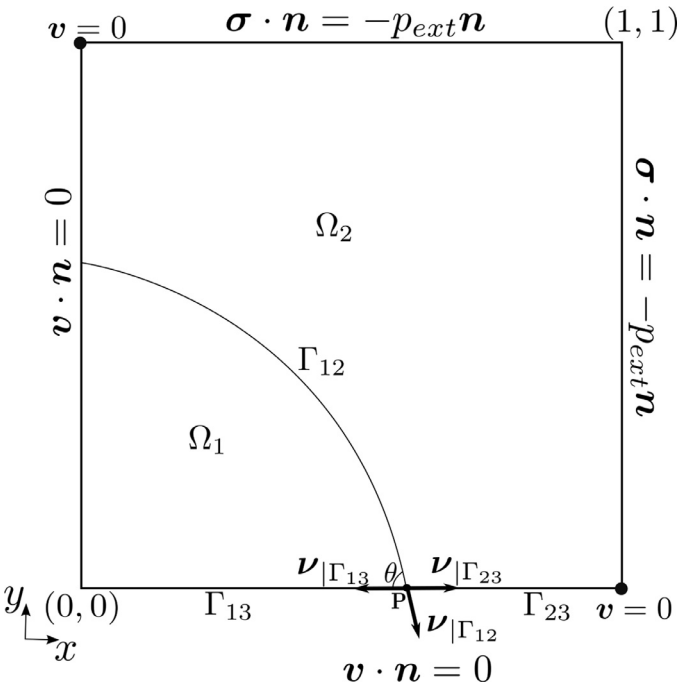

Fig. 1. Schematic of the computational domain $\Omega = \Omega_1 \cup \Omega_2$. The boundary $\partial\Omega$ is divided into two distinct parts, $\partial\Omega = \Gamma_D \cup \Gamma_N$. In this 2D-case, $\Gamma_N = \{y = 1\}$, and $\Gamma_D = \partial\Omega \backslash \Gamma_N$.

Both media Ω_1 and Ω_2 are assumed to behave as incompressible Newtonian fluids of viscosities η_1 and η_2, respectively, with $\eta_2 \ll \eta_1$. Neglecting inertial effects, momentum balance and incompressibility lead to Stokes' equations, expressed in terms of velocity $\boldsymbol{v}$ and pressure p, and governing the flow into $\Omega = \Omega_1 \cup \Omega_2$:

$$\nabla \cdot \boldsymbol{\sigma} = -\boldsymbol{b} \quad \Leftrightarrow \quad \nabla \cdot (2\eta \dot{\boldsymbol{\varepsilon}}(\boldsymbol{v})) - \nabla p = -\boldsymbol{b} \text{ in } \Omega, \tag{1}$$

and

$$\nabla \cdot \boldsymbol{v} = 0 \text{ in } \Omega \tag{2}$$

In momentum balance (1), $\boldsymbol{\sigma}$ is the Cauchy stress tensor[1], η the global viscosity field, $\boldsymbol{b}$ represents the body forces (*e.g.* gravity), all these quantities being associated with the ith fluid in Ω_i. The strain rate tensor $\dot{\boldsymbol{\varepsilon}}(\boldsymbol{v})$ is defined as the symmetric part of the velocity gradient, $\dot{\boldsymbol{\varepsilon}}(\boldsymbol{v}) = \frac{1}{2}(\nabla \boldsymbol{v} + (\nabla \boldsymbol{v})^T)$.

This bifluid Stokes' system is closed when considering boundary conditions. As shown in Fig. 1, two types of conditions will be assumed in the simulations presented. Let us divide the boundary of the computational domain into two parts, Γ_D and Γ_N: $\partial\Omega = \Gamma_D \cup \Gamma_N$ and $\Gamma_D \cap \Gamma_N = \emptyset$. The stress vector is imposed over the boundary Γ_N through a Neumann condition: $\boldsymbol{\sigma} \cdot \boldsymbol{n} = -p_{ext}\boldsymbol{n}$, where p_{ext} is a scalar (the external pressure), and $\boldsymbol{n}$ the outward normal to Γ_N. Over Γ_D, the normal velocity is imposed as zero (Dirichlet condition), except at the two ends of Γ_D where $\boldsymbol{v} = \boldsymbol{0}$ is considered. These ends are the two points (0,1) and (1,0) shown in Fig. 1. More generally, we write that $\boldsymbol{v} = \boldsymbol{0}$ on $\partial\Gamma_D$. The reason of this special condition appears when establishing the weak formulation of the mechanical problem: it allows to remove the corresponding boundary terms that result from the integration by part of the capillary terms.

However, this Stokes' system is physically irrelevant without taking into account additional mechanical equilibrium conditions.

[1] Here and in the following, all vectors and tensors are written in bold font.