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Direct numerical simulations of thermocapillary migration of a droplet attached to a solid wall

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ABSTRACT

This paper is designated to gain further insight into the physical mechanisms of thermal droplet actuation on a wall through direct numerical simulation. Classical theory states that free droplets in a nonuniform temperature field always move towards the hot side. However, when attaching a droplet to a wall with a nonuniform temperature gradient, lubrication theory explains how such a droplet moves towards the colder side. This paper aims at further investigating and clarifying the physical mechanisms and acting forces in the environment of a nonuniform temperature field and offers some explanations. For the numerical simulations of a droplet attached to a wall with a linear temperature gradient and larger contact angles, the full Navier–Stokes equations and energy equation are solved in a Volume of Fluid framework. The solver is extended with a dynamic contact angle treatment and thoroughly validated. The droplet motion is studied both in two and three dimensions, where a movement towards the cold and the warm side can be observed. The forces acting in such a setting are identified and interpreted. A decomposition of the jump conditions shows that the tangential stress due to the temperature dependent surface tension alone would lead to a motion towards the cold side, whereas the normal component alone would move the droplet to the opposite direction. The differences between two- and three-dimensional simulations show that the problem at hand is clearly three-dimensional.

Introduction

Droplet actuation is attracting widespread attention because of its promising potential in droplet-based devices developed for various applications in industry (Darhuber and Troian, 2005). Small droplets attached to a substrate can be actuated by numerous effects, including thermal, chemical, electrochemical, electrical, etc. forces. Such actuated droplets are of special interest in microgravity environments due to the lack of gravitational forces as the driving mechanisms. Despite this relevance, not all physical effects are fully understood, especially in the context of contact line dynamics. In the present work, the temperature dependence of the surface tension is used as the driving force for the droplet movement. This effect is called thermal Marangoni stress.

The movement of small droplets under the influence of gravity and inhomogeneous temperature has been studied for nearly a century. Fedosov derived the stationary velocity of a rising droplet due to a linear temperature field in 1948 in his PhD Thesis, which was published in 1956 in a Russian journal (Fedosov, 1956) and only translated recently (Fedosov, 2013). In Young et al. (1959), Young, Goldstein and Block derived the well known steady migration velocity of a droplet under the influence of gravity and a temperature gradient. Since then, droplet migration has been the subject of numerous analytical, numerical and experimental parameter studies concerning the influence of physical quantities on the steady migration velocity (see e.g. Subramanian and Balasubramaniam, 2001; Haj-Hariri et al., 1997; Nas and Tryggvason, 2003; Ma and Bothe, 2011; Hadland et al., 1999; Thompson et al., 1980). In all these studies, it is accepted that the droplet always moves towards the hot region. This is supported by analytical solutions for the velocity field in cases when a Stokes flow can be assumed (Fedosov, 2013; Young et al., 1959).

However, attaching such a droplet to a wall with a linear lateral temperature gradient, the droplet migrates mostly towards the cold side as stated in Darhuber and Troian (2005). Only very recently a numerical study showed that for large contact angles, such an attached droplet can also migrate towards the hot side. A thorough overview including thermal droplet actuation for experimental, analytical and numerical studies up to 2005 can be found in Darhuber and Troian

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(2005). So far, most investigations, including experimental studies, covered only the parameter set where the droplet moves towards the cold region, namely fluid pairings which exhibit small contact angles. In this region, where lubrication theory is valid, analytical, experimental, and numerical studies show that the droplet either moves to the cold side or does not move at all (see e.g. Gomba and Homsy, 2010; Smith, 1995). The latter case may appear depending on the foot length of the droplet and the magnitude of the temperature gradient as shown in Pratap et al. (2008).

Numerical solutions of the full Navier–Stokes equations for a migrating droplet attached to a wall were only done within the last few years, opening a new field. Tseng et al. conducted in Tseng et al. (2004) three-dimensional simulations, additionally to their experiments. They studied contact angles smaller than 90°, but did not obtain quantitative agreement between their simulations and experiments. In the work of Nguyen and Chen (2010), droplet migration on a wall for squalane and silicon oil droplets was studied in two dimensions for larger contact angles with an extended FEM Solver (COMSOL Multiphysics®). Although an interesting study, they apparently neglected the interfacial gradient of the surface tension in the momentum jump condition which should influence the movement significantly. Only very recently, Sui (2014) tackled the question if droplets attached to a wall with a lateral temperature gradient can migrate towards both sides. He found that they can indeed move towards the cold or hot region, or even not move at all, depending on the contact angle and the viscosity ratio between inner and outer fluid. Furthermore, he studied the influence of contact angle hysteresis. His simulations are all two-dimensional. For a comparison to experiments, which has yet to be conducted for larger contact angles, fully three-dimensional simulations are currently missing. Moreover, to obtain the desired deeper understanding of the direction-change, a numerical algorithm that is capable of accurately capturing the multiphysics, especially contact line dynamics and variable surface tension, is mandatory.

The numerical studies in the present work are carried out with the Volume of Fluid in-house code Free Surface 3D (FS3D) with piecewise linear interface reconstruction (PLIC,[20]). The thermocapillary forces are determined as in Ma and Bothe (2011). The contact angle at the wall is ensured by an appropriate boundary condition, including the normal vectors and the curvature calculation. Within the employed balanced CSF model (Francois et al., 2006; Renardy and Renardy, 2002), the curvature is determined via a height function algorithm (Popinet, 2009). Thus, the height functions are altered in such a way that the contact angle is matched, where the dynamic contact angle is determined with Kistler's correlation ((Berg, 1993), Chapter 6). The stress singularity at the contact line is relaxed by the inherent slip of the employed staggered grid as discussed before in Renardy et al. (2001). Since this slip is mesh dependent and the empirical correlation valid on a larger scale than the grid size, a similar approach to the one by Afkhami et al. (2009) is used. In imitation of hydrodynamic theory, where different regions and corresponding contact angles are defined, the macroscopic dynamic contact angle is transformed to the smaller grid scale. In this way, the large slip length and thereby large contact line velocity is counteracted. In addition, this algorithm contradicts the strong mesh dependency of the simulation results. For wider overviews on contact line dynamics we refer to the books and reviews (Berg, 1993; Shikhmurzaev, 2007; Sui et al., 2014; Blake, 2006) and to the numerous references given there.

Employing this extended solver, the influence of different physical parameters on the droplet behavior is studied. An in-depth look at the acting forces and physical mechanisms allows a deeper physical understanding of the droplet behavior. Apparently for the first time, three-dimensional simulations of thermal droplet migration on a wall for large contact angles are done and compared to two-dimensional results.

Mathematical and numerical model

Governing equations

We consider incompressible two-phase flow of immiscible Newtonian fluids with a variable surface tension for the deformable interface and additional heat transfer. The mathematical model applied in this work is based on continuum mechanics and employs a sharp interface, i.e. the deformable and moving interface between the two phases is assumed to have zero thickness. The resulting two-phase model consists of two sets of equations in the bulk phases and additional transmission conditions at the interface.

Inside the phases, the continuity and (incompressible) Navier–Stokes equations hold, expressing the balance of mass and momentum. The temperature is determined by solving the temperature form of the energy balance equation. In addition, appropriate jump conditions have to be formulated to complement the balances of mass, momentum and energy. To formulate these jump conditions, we denote the liquid phase by the superscript l and the continuous gas phase by g. We assume that there is no slip between the phases at the interface so that the tangential velocities are continuous, and since no phase change is bound to happen and the interface does not have mass in this model, the normal velocities are also continuous. This results in the following set of equations:

$$\nabla \cdot \mathbf{u} = 0, \qquad \text{in } \Omega \setminus \Sigma \tag{1}$$

$$\partial_t(\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) = -\nabla p + \nabla \cdot \mathbf{S} + \mathbf{g}\rho, \qquad \text{in } \Omega \setminus \Sigma \tag{2}$$

$$\partial_t(\rho c_p T) + \nabla \cdot (\rho c_p T \mathbf{u}) = \nabla \cdot (\lambda \nabla T) + \mathbf{S} : \nabla \mathbf{u}, \qquad \text{in } \Omega \setminus \Sigma \tag{3}$$

$$[[\mathbf{u}]] = 0, \qquad \text{on } \Sigma \tag{4}$$

$$[[p\mathbf{I} - \mathbf{S}]] \cdot \mathbf{n}_\Sigma = \sigma \kappa \mathbf{n}_\Sigma + \sigma_T \nabla_\Sigma T, \qquad \text{on } \Sigma \tag{5}$$

$$[[\lambda \nabla T]] \cdot \mathbf{n}_\Sigma = 0 \qquad \text{on } \Sigma. \tag{6}$$

Here $\mathbf{S} = \mu[\nabla \mathbf{u} + (\nabla \mathbf{u})^\mathsf{T}]$ denotes the viscous stress tensor, $\mathbf{u}$ the velocity, T the temperature, ρ the density, p the pressure, g the acceleration of gravity, c_p heat capacity, and λ the thermal conductivity. The temperature dependence of the surface tension σ is given by the linear relationship known as the Eötvös rule, i.e.

$$\sigma(T) = \sigma_0 + \sigma_T(T - T_0), \tag{7}$$

where the temperature coefficient $\sigma_T = \partial\sigma/\partial T$ of the surface tension is negative as it is for most common liquids. Above, $[[\phi]]$ denotes the jump of a quantity ϕ at the interface if the latter is crossed against the surface normal $\mathbf{n}_\Sigma$.

When the fluid/liquid-interface is in contact with a solid surface, the tangent planes form a contact angle θ at the contact line. In the absence of external forces, the surface forces parallel to the wall acting at the contact line are in balance, i.e.

$$\sigma_{s,f} = \sigma_{s,l} + \sigma_{f,l} \cos\theta_e. \tag{8}$$

Here θ_e denotes the equilibrium contact angle, $\sigma_{s,l}$ the surface tension between the solid phase and the liquid, $\sigma_{s,f}$ the surface tension between the solid phase and a fluid and $\sigma_{f,l} = \sigma$. Eq. (8) is the well-known Young's equation.

One-field formulation

For the numerical solution in the Volume of Fluid (VOF) context, an one-field formulation of the two-phase model is required, containing only a single set of equations valid in both phases and at the