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# Direct numerical simulation of variable surface tension flows using a Volume-of-Fluid method

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ABSTRACT

We develop a general methodology for the inclusion of a variable surface tension coefficient into a Volume-of-Fluid based Navier–Stokes solver. This new numerical model provides a robust and accurate method for computing the surface gradients directly by finding the tangent directions on the interface using height functions. The implementation is applicable to both temperature and concentration dependent surface tension coefficient, along with the setups involving a large jump in the temperature between the fluid and its surrounding, as well as the situations where the concentration should be strictly confined to the fluid domain, such as the mixing of fluids with different surface tension coefficients. We demonstrate the applicability of our method to the thermocapillary migration of bubbles and the coalescence of drops characterized by a different surface tension coefficient.



## 1. Introduction

Flows induced by the spatial variations in the surface tension coefficient, also known as the Marangoni effect [1], can be caused by surfactants, temperature or concentration gradients, or a combination of these effects. Understanding these flows is important since they are relevant in microfluidics [2], heat pipe flows [3], motion of drops or bubbles in materials processing applications that include heating or cooling [4], evolution of metal films of nanoscale thickness melted by laser pulses [5,6], and in a variety of other thin film flows, see [7,8] for reviews.

Numerical methods for studying variable surface tension flows include front tracking [9], level set [10], diffuse interface [11], marker particle [12,13], immersed boundary [14], boundary integral [15], interface-interaction [16], and Volume-of-Fluid (VOF) [17–19] methods. The VOF method is efficient and robust for tracking the topologically complex evolving interfaces. The improvements in the recent years in the computation of the surface tension force have empowered the VOF method to become a widespread method for modeling interfacial flows [20,21]. However, an accurate implementation of the variable surface tension coefficient in the VOF formulation is still lacking a general treatment.

A challenge of including the variable surface tension effects into the VOF method is that the surface tension coefficient is not known exactly at the interface — only the value averaged over a computational cell containing the interface is known. To obtain the surface tension coefficient at the interface, an approximation from the values near the interface, usually calculated at the center of each adjacent computational cell, is necessary. As we outline below, the approximation of the

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interface values has been carried out in the literature differently, depending on the physics of the problem studied. An additional major issue concerns computing the surface gradients of the surface tension coefficient.

In Alexeev et al. [22] and Ma and Bothe [19], the VOF method is used to study flows involving a temperature dependent surface tension coefficient. The implementation in Alexeev et al. [22] solves the heat equation in fluids on both sides of the interface, and then imposes the continuity of the temperature and flux at the interface, and the conservation of energy in the cell containing the interface to approximate the temperature in the fluid and air in the cell. These temperature values are then used to calculate surface gradients of the temperature from nearby cells that are not cut by the interface; these gradients are then exponentially extrapolated to the interface. In the work by Ma and Bothe [19], the temperature at the interface is approximated from the temperatures in the liquid and the gas by imposing the continuity of the heat flux at the interface. The surface gradients of the temperature are approximated by computing the derivatives in each coordinate direction using finite differences, and then projecting them onto the tangential direction. If the interface is not contained in all cells of the finite difference stencil, then one sided differences are used. Hence, this method requires the temperature solution on both sides of the interface and therefore cannot be used for the setups involving a large difference in thermal conductivity of the two fluids, since the fluids may have a large difference in the temperature. Furthermore, both of these methods are not applicable to setups where the surface tension only depends on the concentration, such as mixing of miscible liquids with a different surface tension coefficient. In the work by James and Lowengrub [18], the VOF method is used to study the flows induced by the surfactant concentration gradient. In their method, the concentration values at the interface are obtained by imposing the condition that the average concentration at the interface is equal to the average concentration in the cell containing the interface. Then, the surface gradients are computed using the cell-center interfacial concentration in the two adjacent cells.

Here, we develop a method that can be applied to both temperature and concentration dependent surface tension coefficient, with the surface gradients computed using the cell-center values in the interfacial cells only. We note that comparing to the methods by Alexeev et al. [22] and Ma and Bothe [19], our approach is simpler, while retaining the accuracy, in that it uses interfacial cells only to compute the temperature at the interface, while these existing methods use interpolation around the interface for liquid and air temperature. We find the tangential gradients directly by computing the tangent directions on the interface using height functions [23]. We therefore note that our numerical method is consistent with underlying height-function method used for computing the surface tension force in the original method in [23].

Another advantage of our numerical method is its ability to naturally and automatically handle the surface tension variation that may result from either thermal or concentration gradients. Our method can therefore seamlessly be applied to the setups involving the concentration confined to the fluid domain, e.g. mixing of liquids with a different surface tension coefficients, as well as the configurations involving a large jump of the temperature between the liquid and the surrounding.

Our numerical method is implemented using Gerris: an open source adaptive Navier–Stokes solver [24,23]. The current version includes Continuum Surface Force (CSF) [25] implementation of the surface tension force with height function algorithm for computing the interfacial normal and curvature [23]. Here, we present a method for extending this formulation to include a variable surface tension coefficient, allowing to consider the surface force in the direction tangential to the interface. As far as we are aware, this is the first implementation of the variable surface tension combined with the accurate implementation of the CSF method, such that the curvature and interface normals are computed using generalized height functions [23]. In addition, we demonstrate that our new numerical method results in second order accurate computation of the surface tension gradients in the tangential direction which is a key element for describing the variable surface tension problems accurately. Such a result has not yet been reported in the literature. With the above mentioned improvements, our extension is a step closer to cover all aspects of the variable surface tension flows; the remaining one is the implementation of the surfactant transport and the surface tension gradients due to the presence of the surfactants. This will be a topic of our future work.

The rest of this paper is organized as follows: Section 2 gives an overview of the VOF method, including the CSF method for the computation of the surface tension; Section 3 describes in detail the implementation of the variable surface tension coefficient in two and three dimensions; and Section 4 illustrates the performance of our method for various test cases, including temperature and concentration dependent surface tension.

## 2. Governing equations

We consider an incompressible two-phase flow described by the Navier–Stokes equations

$$\rho(\partial_t \mathbf{u} + \mathbf{u}\cdot\nabla\mathbf{u}) = -\nabla p + \nabla\cdot(2\mu D) + \mathbf{F}, \tag{1}$$

$$\nabla\cdot\mathbf{u} = 0, \tag{2}$$

and the advection of the phase-dependent density $\rho(\chi)$

$$\partial_t \rho + (\mathbf{u}\cdot\nabla)\rho = 0, \tag{3}$$

where $\mathbf{u} = (u, v, w)$ is the fluid velocity, $p$ is the pressure, $\rho(\chi) = \chi\rho_1 + (1-\chi)\rho_2$ and $\mu(\chi) = \chi\mu_1 + (1-\chi)\mu_2$ are the phase dependent density and viscosity respectively, and $D$ is the rate of deformation tensor $D = \left(\nabla\mathbf{u} + \nabla\mathbf{u}^T\right)/2$. Subscripts 1 and 2 correspond to the fluids 1 and 2, respectively (see Fig. 1). Here, $\chi$ is the characteristic function, such that $\chi = 1$ in