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Numerical simulation of single droplet dynamics in three-phase flows using ISPH

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ABSTRACT

In this study, a new surface tension formulation for modeling incompressible, immiscible three-phase fluid flows in the context of incompressible smoothed particle hydrodynamics (ISPH) in two dimensions has been proposed. A continuum surface force model is employed to transform local surface tension force to a volumetric force while physical surface tension coefficients are expressed as the sum of phase specific surface tension coefficients, facilitating the implementation of the proposed method at triple junctions where all three phases are present. Smoothed color functions at fluid interfaces along with artificial particle displacement throughout the computational domain are combined to increase accuracy and robustness of the model. In order to illustrate the effectiveness of the proposed method, several numerical simulations have been carried out and results are compared to analytical data available in literature. Results obtained by simulations are compatible with analytical data, demonstrating that the ISPH scheme proposed here is capable of handling three-phase flows accurately.

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1. Introduction

Multiphase flows where two or more fluids have interfacial contact surfaces are one of the most common features observed in many engineering and natural processes and have been a subject of interest for modeling in many computational fluid dynamics (CFD) studies. It is indeed a challenging problem as the evolution of the interface is a crucial step in modeling of multiphase flows which needs to be handled delicately to result in reliable simulations.

In their simplest form, multiphase flows are composed of two immiscible fluid streams. Many studies have been performed on two-phase flows using mesh dependent, meshless and hybrid approaches. Mesh dependent methods include Volume of Fluid (VOF) [1–3], Level Set (LS) [4–6] and Phase Field methods [7,8] where the interface is captured implicitly through use of a scalar function. These methods are also referred to as Eulerian approaches. Hybrid Eulerian–Lagrangian approaches, such as the Front Tracking method [9,10], provide a sharper interface representation by employing markers to track the interface explicitly, which adds to their accuracy at the cost of extra complexity and computational expense. In this regard, the Lagrangian nature of meshless methods is an inherent advantage of this kind of approach as it facilitates the tracking of interfaces with large deformations. Among all different variants of meshless methods, Smoothed Particle Hydrodynamics (SPH) has received a great deal of attention in modeling multiphase flows [11–18].

Despite the large pool of research available in two-phase flows, there have been relatively fewer studies carried out on flows containing three different fluids, partly due to complexities inherent in phase interactions and possible triple-junctions present in these flows. A few examples include level set studies of triple junctions [19,20] and droplet spreading [21],

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droplet impact simulation using front tracking [22], phase field simulations of several three-phase flows [23,24] and weakly compressible smoothed particle hydrodynamics simulations of two- and three-phase flows [25].

In this study, an incompressible SPH (ISPH) scheme based on the projection method initially proposed by Cummins and Rudman [26] is developed to simulate two-dimensional immiscible three-phase flows. Surface tension forces are taken into consideration using the Continuum Surface Force (CSF) model proposed by Brackbill et al. [27]. In order to capture the interaction between different phases, the surface tension coefficient decomposition method proposed in Smith et al. [20] has been employed. A number of test cases have been simulated to test the capabilities of the proposed scheme in a methodical manner. First, elongation of a circular droplet encompassed between two immiscible fluid layers have been studied and compared to analytic values. Extending this test case towards a more dynamic one, levitation of a circular droplet initially at rest between two layers of immiscible fluids have been simulated. Finally to demonstrate flexibility of the method in handling moving contact lines involving density and viscosity differences, simulations of droplet spreading on a solid surface are conveyed and compared against analytical results available in literature.

The outline of this paper is as follows. Mathematical formulation along with numerical approximations employed are presented in Sections 2 and 3. Results of the simulations and validations against literature data are presented and discussed in Section 4 and concluding remarks are drawn in Section 5.

2. Mathematical formulation

Mass and momentum conservation equations for an incompressible flow may be written as

$$\nabla \cdot \mathbf{u} = 0, \tag{1}$$

$$\rho \frac{\mathrm{D}\mathbf{u}}{\mathrm{D}t} = -\nabla p + \nabla \cdot \boldsymbol{\tau} + \mathbf{f}_{(b)} + \mathbf{f}_{(s)}, \tag{2}$$

where $\mathbf{u}$ is the velocity vector, p is pressure, ρ is density, t is time and $\mathrm{D}/\mathrm{D}t = \partial/\partial t + u^k \partial/\partial x^k$ represents the material time derivative. Here, $\boldsymbol{\tau}$ and $\mathbf{f}_{(b)}$ are viscous stress tensor and body forces exerted on the flow, respectively. While the body force is taken to be $\rho\mathbf{g}$ where $\mathbf{g}$ is gravitational acceleration, the viscous stress tensor is defined as

$$\boldsymbol{\tau} = \mu \left(\nabla\mathbf{u} + (\nabla\mathbf{u})^T \right), \tag{3}$$

where superscript T represents the transpose operation. For the sake of computational simplicity and efficiency, it is preferable to express the local surface force as an equivalent volumetric force, $\mathbf{f}_{(s)}$, according to the Continuum Surface Force (CSF) method originally proposed by Brackbill et al. [27]. Replacing the sharp interface between two fluids with a transitional region of finite thickness through multiplication of local surface tension force with a one-dimensional Dirac delta function [28], δ, surface tension force may be formulated as

$$\mathbf{f}_{(s)} = \sigma \kappa \hat{\mathbf{n}} \delta. \tag{4}$$

Here, surface tension coefficient, σ, is taken to be constant while κ represents interface curvature, $-\nabla \cdot \hat{\mathbf{n}}$, where $\hat{\mathbf{n}}$ is unit surface normal vector.

The above definition for volumetric surface tension force has to be developed further if it is to be used for a three-phase flow as a fluid particle may be affected by more than two interfaces simultaneously, which is the case near triple junctions where all three phases meet. In order to circumvent this difficulty, Smith et al. [20] have proposed decomposing the surface tension coefficient into phase specific surface tension coefficients such that $\sigma^{\alpha\beta} = \sigma^\alpha + \sigma^\beta$. Here, $\sigma^{\alpha\beta}$ is the physical surface tension coefficient between phases α and β while σ^α and σ^β are phase specific surface tension coefficients for αth and βth phases, respectively. Considering a three-phase flow, the aforementioned decomposition will lead to the following relations for phase specific surface tension coefficients,

$$\begin{cases} \sigma^1 = 0.5 \left(\sigma^{12} + \sigma^{13} - \sigma^{23} \right), \\ \sigma^2 = 0.5 \left(\sigma^{12} - \sigma^{13} + \sigma^{23} \right), \\ \sigma^3 = 0.5 \left(-\sigma^{12} + \sigma^{13} + \sigma^{23} \right). \end{cases} \tag{5}$$

Combining phase specific surface tension coefficients defined above with (4), the resultant volumetric surface tension force may be rewritten as a sum of three force components as

$$\mathbf{f}_{(s)} = \sum_{\alpha=1}^{3} \left(\sigma \kappa \hat{\mathbf{n}} \delta \right)^\alpha. \tag{6}$$

To be able to distinguish different fluids of the three-phase flow of interest, three concurrent color functions are introduced where each one is associated to a certain phase. Thus the color function for phase α, $\hat{c}^\alpha$, has a value of one where phase α is present while other color functions are set to zero. Interface curvature, unit normals and surface tension forces related to each phase are computed using its corresponding color function and will be discussed further in the following section.

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